

=>



100.0% PROCESSED 7813 ITERATIONS 123 ANSWERS
SEARCH TIME: 00.00.01

L7 123 SEA SSS FUL L5

=> s 17
L8 39 L7

=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 39 ANSWERS - CONTINUE? Y/(N):y

=>



chain nodes :
1 2 3 4 5 6 7 8 9 11 12
chain bonds :
1-2 1-12 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-11
exact/norm bonds :
6-7 7-8
exact bonds :
1-2 1-12 2-3 3-4 4-5 5-6 8-9 9-11

G1:Cb,Cy,Hy

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 11:CLASS 12:CLASS

L1 STRUCTURE UPLOADED

=> s 11 sss sam
SAMPLE SEARCH INITIATED 10:27:34 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 72 TO ITERATE

100.0% PROCESSED 72 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 931 TO 1949
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> s 11 sss full
FULL SEARCH INITIATED 10:27:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1651 TO ITERATE

100.0% PROCESSED 1651 ITERATIONS 44 ANSWERS
SEARCH TIME: 00.00.01

L3 44 SEA SSS FUL L1

=> s 13
L4 11 L3

=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 11 ANSWERS - CONTINUE? Y/(N):y

=>



chain nodes :
1 2 3 4 5 6 7 9
chain bonds :
1-2 1-9 2-3 3-4 4-5 5-6 6-7
exact/norm bonds :
1-9 4-5 5-6
exact bonds :
1-2 2-3 3-4 6-7

G1:Cb,Cy,Hy

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 9:CLASS

L1 STRUCTURE UPLOADED



```

=> s 11 sss sam
SAMPLE SEARCH INITIATED 12:55:09 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 623 TO ITERATE

100.0% PROCESSED 623 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH **COMPLETE**
PROJECTED ITERATIONS: 10963 TO 13957
PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s 11 sss full
FULL SEARCH INITIATED 12:55:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 11729 TO ITERATE

100.0% PROCESSED 11729 ITERATIONS 53 ANSWERS
SEARCH TIME: 00.00.01

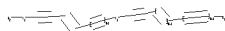
L3 53 SEA SSS FUL L1

=> s 13
L4 20 L3

=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 20 ANSWERS - CONTINUE? Y/(N):y

=>

```



```

chain nodes :
2 3 4 5 6 7 8 9 10 11 12 13 14 15 20 24
chain bonds :
2-3 2-24 3-4 4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14 14-15 15-20
exact/norm bonds :
2-3 2-24 8-9 9-10 15-20
exact bonds :
3-4 4-5 5-6 6-7 7-8 10-11 11-12 12-13 13-14 14-15

```

G1:Cb,Cy,Hy

G2:C,H,O,N,Cl,Br,F,I

G3:C,H,Si,Cb,Cy,Hy

Match level :
2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 20:CLASS 24:CLASS

```

L5 STRUCTURE UPLOADED

=> s 15 sss full
FULL SEARCH INITIATED 13:07:29 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 11729 TO ITERATE

100.0% PROCESSED 11729 ITERATIONS 106 ANSWERS
SEARCH TIME: 00.00.01

L6 106 SEA SSS FUL L5

=> s 16
L7 32 L6

=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 32 ANSWERS - CONTINUE? Y/(N):y

=>

```



```

chain nodes :
4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20
chain bonds :
4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 13-14 14-15 15-16 16-17 17-18 18-19 19-20
exact/norm bonds :
4-5 5-6 11-12 12-13 18-19 19-20
exact bonds :
6-7 7-8 8-9 9-10 10-11 13-14 14-15 15-16 16-17 17-18

```



G1:Cb,Cy,Hy

G2:C,H,O,N,Cl,Br,F,I

G3:C,H,Si,Cb,Cy,Hy

Match level :

4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS

L8 STRUCTURE UPLOADED

=> s 18 sss full

FULL SEARCH INITIATED 13:20:23 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 11728 TO ITERATE

100.0% PROCESSED 11728 ITERATIONS

70 ANSWERS

SEARCH TIME: 00.00.01

L9 70 SEA SSS FUL L8

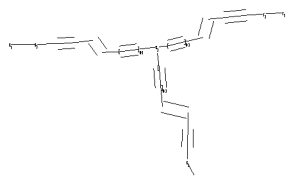
=> s 19

L10 22 L9

=> d ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 22 ANSWERS - CONTINUE? Y/(N):y

=>



chain nodes :

4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 26 27 28 29 30 31 32 33

chain bonds :

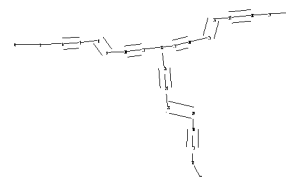
4-5 5-6 6-7 7-8 8-9 9-10 10-11 11-12 12-13 12-26 13-14 14-15 15-16 16-17 17-18 18-19 19-20 26-27 27-28 28-29 29-30 30-31 31-32 32-33

exact/norm bonds :

4-5 5-6 11-12 12-13 12-26 18-19 19-20 31-32 32-33

exact bonds :

6-7 7-8 8-9 9-10 10-11 13-14 14-15 15-16 16-17 17-18 26-27 27-28 28-29 29-30 30-31



G1:Cb,Cy,Hy

G2:C,H,O,N,Cl,Br,F,I

G3:C,H,Si,Cb,Cy,Hy

Match level :

4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 26:CLASS 27:CLASS

28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS

L11 STRUCTURE UPLOADED

=> s 111 sss full

FULL SEARCH INITIATED 13:30:22 FILE 'REGISTRY'

SCREENING

FULL SCREEN SEARCH COMPLETED - 11407 TO ITERATE

100.0% PROCESSED 11407 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.34

L12 2 SEA SSS FUL L11

=> s 112

L13 2 L12

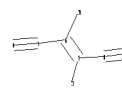
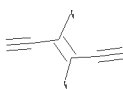
=> d ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 2 ANSWERS - CONTINUE? Y/(N):y

=>

FILE 'HOME' ENTERED AT 15:53:37 ON 18 DEC 2009

=>



```
chain nodes :
4 5 6 7 8 9 10 11
chain bonds :
4-5 5-6 6-7 6-10 7-8 7-11 8-9
exact/norm bonds :
6-10 7-11
exact bonds :
4-5 5-6 6-7 7-8 8-9
```

G1:Cb,Cy,Hy

G2:C,H,O,N,Cl,Br,F,I

G3:C,H,Si,Cb,Cy,Hy

G4:H,Ak

Match level :

4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS

L1 STRUCTURE UPLOADED

```
=> s 11 sss full
FULL SEARCH INITIATED 15:54:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 7813 TO ITERATE
```

```
100.0% PROCESSED 7813 ITERATIONS 3088 ANSWERS
SEARCH TIME: 00.00.01
```

L2 3088 SEA SSS FUL L1

=> s 12

L3 814 L2

=> 13 and (electroluminescence or electroluminescent or luminescent or (light emitting) or OLED)

```
26473 ELECTROLUMINESCENCE
30 ELECTROLUMINESCENCES
26478 ELECTROLUMINESCENCE
(ELECTROLUMINESCENCE OR ELECTROLUMINESCENCES)
5 ELECTROLUMINESCENSE
26479 ELECTROLUMINESCENCE
(ELECTROLUMINESCENCE OR ELECTROLUMINESCENSE)
90044 ELECTROLUMINESCENT
8 ELECTROLUMINESCENTS
90047 ELECTROLUMINESCENT
(ELECTROLUMINESCENT OR ELECTROLUMINESCENTS)
65004 LUMINESCENT
10 LUMINESCENTS
65010 LUMINESCENT
(LUMINESCENT OR LUMINESCENTS)
1334311 LIGHT
12618 LIGHTS
1338549 LIGHT
(LIGHT OR LIGHTS)
140113 EMITTING
219 EMITTINGS
140157 EMITTING
(EMITTING OR EMITTINGS)
76113 LIGHT EMITTING
(LIGHT(W)EMITTING)
7493 OLED
3722 OLEDs
9385 OLED
(OLED OR OLEDs)
```

L4 3 L3 AND (ELECTROLUMINESCENCE OR ELECTROLUMINESCENT OR LUMINESCENT OR (LIGHT EMITTING) OR OLED)

```
=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/(N):y
```

=> 13 and (electroluminescence or electroluminescent or luminescent or (light emitting) or OLED or (non linear optics) or NLO)

```
26473 ELECTROLUMINESCENCE
30 ELECTROLUMINESCENCES
26478 ELECTROLUMINESCENCE
(ELECTROLUMINESCENCE OR ELECTROLUMINESCENCES)
5 ELECTROLUMINESCENSE
26479 ELECTROLUMINESCENCE
(ELECTROLUMINESCENCE OR ELECTROLUMINESCENSE)
90044 ELECTROLUMINESCENT
8 ELECTROLUMINESCENTS
90047 ELECTROLUMINESCENT
(ELECTROLUMINESCENT OR ELECTROLUMINESCENTS)
65004 LUMINESCENT
10 LUMINESCENTS
65010 LUMINESCENT
(LUMINESCENT OR LUMINESCENTS)
1334311 LIGHT
12618 LIGHTS
1338549 LIGHT
(LIGHT OR LIGHTS)
140113 EMITTING
219 EMITTINGS
140157 EMITTING
(EMITTING OR EMITTINGS)
76113 LIGHT EMITTING
```

```

(LIGHT(W)EMITTING)
7493 OLED
3722 OLEDs
9385 OLED
(OLED OR OLEDs)
1110208 NON
38 NONs
1110237 NON
(NON OR NONs)
710357 LINEAR
74 LINEARS
710397 LINEAR
(LINEAR OR LINEARS)
53122 OPTICS
311 NON LINEAR OPTICS
(NON(W)LINEAR(W)OPTICS)
7807 NLO
19 NLOS
7820 NLO
(NLO OR NLOS)
L5 6 L3 AND (ELECTROLUMINESCENCE OR ELECTROLUMINESCENT OR LUMINESCENT
OR (LIGHT EMITTING) OR OLED OR (NON LINEAR OPTICS) OR NLO)

=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 6 ANSWERS - CONTINUE? Y/(N):y

=>

```

Connecting via Winsock to STN

Welcome to STN International! Enter x:X

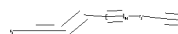
LOGINID:SSPTAKB1794

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

=>



```

chain nodes :
1 2 3 4 5 6 7 8 9 11
chain bonds :
1-2 1-11 2-3 3-4 4-5 5-6 6-7 7-8 8-9
exact/norm bonds :
1-11 6-7 7-8
exact bonds :
1-2 2-3 3-4 4-5 5-6 8-9

```

G1:Cb,Cy,Hy

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:CLASS 9:CLASS 11:Atom

L1 STRUCTURE UPLOADED

=> s 11 sss full

FULL SEARCH INITIATED 12:23:04 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 12029 TO ITERATE

100.0% PROCESSED 12029 ITERATIONS

106 ANSWERS

SEARCH TIME: 00.00.01

L2 106 SEA SSS FUL L1

=> s 12

L3 32 L2

=> d ibib abs hitstr 1-

YOU HAVE REQUESTED DATA FROM 32 ANSWERS - CONTINUE? Y/(N):y

.L3 ANSWER 1 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2009:1099083 CAPLUS Fulltext

Document Number

151:508432

Title

Hybrid Conjugated Organic Oligomers Consisting of Oligodiacetylene and Thiophene Units: Synthesis and Optical Properties

Author/Inventor

Plazak, Gregor S.; van Grujthuisen, Kitty; van Doorn, Reindert H.; van Lagen, Barend; Sudhoelter, Ernst J. R.; Zuilhof, Han

Patent Assignee/Corporate Source

Laboratory of Organic Chemistry, Wageningen University, Dreijenplein 8, Wageningen, 6703 HB, Neth.

Source

Chemistry-A European Journal (2009), 15(36), 9085-9096, S9085/1-S9085/19 CODEN: CEUJED; ISSN: 0947-6539

Document Type

Journal

Language

English

Abstract

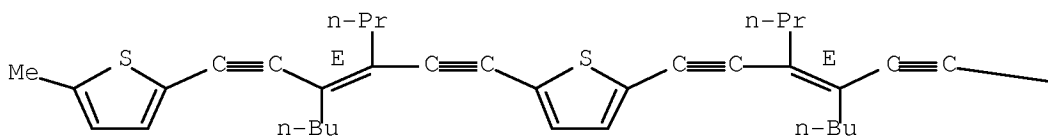
Novel and highly soluble hybrid conjugated organic oligomers consisting of oligodiacylene and thiophene units have been synthesized in high purity through iterative and divergent approaches based on a sequence of Sonogashira reactions. The series of thiophene-containing oligodiacylenes and homocoupled oligodiacylenes show, both in solution and in the solid state, a strong optical absorption, which is progressively red shifted with increasing chain length. The linear correlation of the absorption maximum with the inverse of conjugation length (CL = number of double and triple bonds) shows that the effective conjugation length of this system is extended up to at least CL = 20. Furthermore, absorption measurements of dropcast thin films display not only a bathochromic shift of the absorption maxima but also a higher wavelength absorption, which is attributed to increased π - π interactions. The wavelength of the maximum fluorescence emission also increases with CL, and emission is maximal for oligomers with CL = 7-12 (fluorescence quantum yield Φ_F = approx. 0.2). Both longer and shorter oligomers display marginal emission. The calculated Stokes shifts of these planar materials are relatively large (0.4 eV) for all oligomers, and likely due to excitation to the S₂ state, thus suggesting that the presence of enyne moieties dominates the ordering of the lowest excited states. The fluorescence lifetimes (τ_F) are short (τ_{Fmax} = \approx 1 ns) and closely follow the tendency obtained for the fluorescence quantum yield. The anisotropy lifetimes show a near-linear increase with CL in line with highly rigid oligomers.

Hit Structure

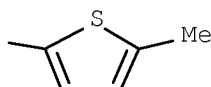
CAS Registry Number
1192820-79-3 CAPLUS

Chemical or Trade Name
Thiophene, 2,5-bis[(3E)-4-[2-(5-methyl-2-thienyl)ethynyl]-3-propyl-3-octen-1-yn-1-yl]- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L3 ANSWER 2 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2009:76616 CAPLUS [Full Text](#)

Document Number

150:167710

Title

Push-pull hyperbranched molecules. A theoretical study

Author/Inventor

Ramos, Estrella; Guadarrama, Patricia; Teran, Gerardo; Fomine, Serguei

Patent Assignee/Corporate Source

Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, Mexico, 04510, Mex.

Source

Journal of Physical Organic Chemistry (2009), 22(1), 9-16 CODEN: JPOCEE; ISSN: 0894-3230

Document Type

Journal

Language

English

Abstract

The electronic properties of the ground state, unrelaxed and relaxed first excited states of push-pull hyperbranched mols. bearing amino and nitro terminal groups have been studied at BB1K/cc-pvdz/HF/6-31g(d), TD-BB1K/cc-pvdz/HF/6-31g(d) and TD-BB1K/cc-pvdz/CIS/6-31g(d) levels of theory, resp. It was demonstrated that dendritic architecture of push-pull mols. favors the charge transfer in the excited state compared to linear mols.

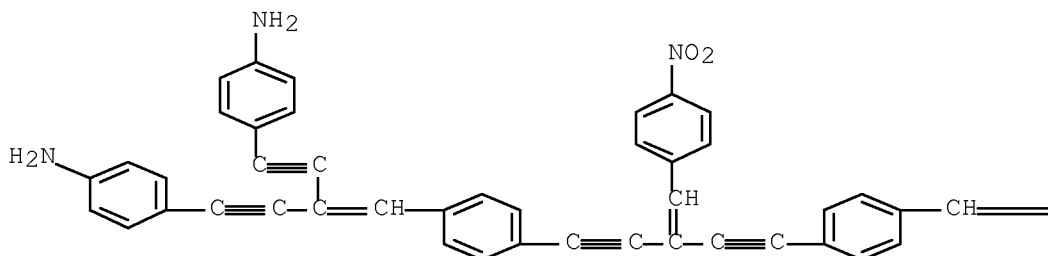
The possibility of adopting a plane conformation is an important condition for the charge transfer in an excited state. According to the calcs. 1:1 ratio of donor and acceptor groups is another important precondition for the manifestation of strong charge separation in the excited state. In case of excess of nitro groups over the amino, some of the excitations participating in the S₀ → S₁ transition favor the charge transfer in the excited state in the opposite directions, thus decreasing the charge separation

Hit Structure

CAS Registry Number
1107616-71-6 CAPLUS

Chemical or Trade Name
Benzenamine, 4,4'-[3-[[4-[5-[4-[4-(4-aminophenyl)-2-[2-(4-aminophenyl)ethynyl]-1-buten-3-yn-1-yl]phenyl]-3-[(4-nitrophenyl)methylene]-1,4-pentadiyn-1-yl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)

PAGE 1-A



Chemical or Trade Name
Benzenamine, 4,4'-[3-[[4-[4-[4-(4-aminophenyl)-2-[2-(4-aminophenyl)ethyl]yl]-1-buten-3-yn-1-yl]phenyl]-3-[[4-[4-[4-(4-nitrophenyl)-2-[2-(4-nitrophenyl)ethyl]yl]-1-buten-3-yn-1-yl]phenyl]-2-[2-[4-(4-nitrophenyl)-2-[2-(4-nitrophenyl)ethyl]yl]-1-buten-3-yn-1-yl]phenyl]ethyl]yl]-1-buten-3-yn-1-yl]phenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)

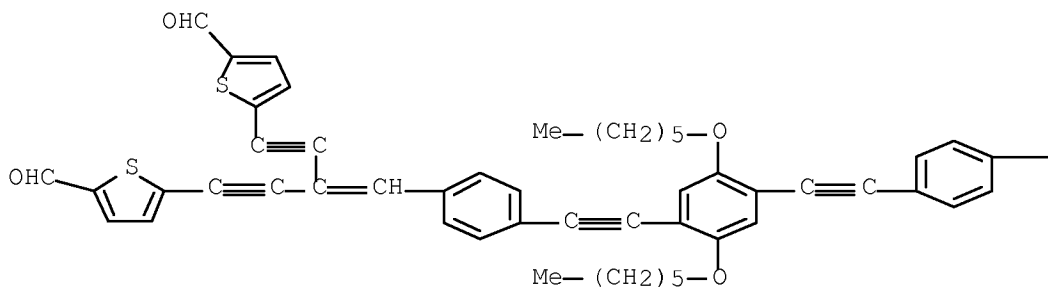
The synthesis of two new tetratfullerene nanoconjugates in which four C₆₀ units are covalently connected through different π -conjugated oligomers (oligo(p-phenylene ethynylene) and oligo(p-phenylene vinylene)) is described. The photovoltaic response of these C₆₀-based conjugates was evaluated by using them as the only active material in organic solar cells, showing a low photovoltaic performance. Photophys. studies in solution demonstrated a very fast (apprx.10 ps) deactivation of the singlet excited state of the central core unit to produce both charge-separated species (i.e., C₆₀^{•-}-oligomer^{•+}-(C₆₀)₃ and C₆₀ centered singlet excited states). The charge-separated state recombines partly to the C₆₀ centered singlet state that undergoes subsequent intersystem crossing. Photophys. studies carried out in films support these data, exhibiting long-lived triplet excited states. For both tetratfullerene arrays, the low yield of long-lived charge carriers in thin films accounts for the limited photovoltaic response. On the contrary, utilizing the oligo(p-phenylene vinylene) centered precursor aldehyde as an electron donor and antennae unit and mixing with the well-known C₆₀ derivative PCBM, the photophys. studies in films show the formation of long-lived charges. The photovoltaic devices constructed from these mixts. showed a relatively high photocurrent of 2 mA/cm². The sharp contrast between the nanoconjugates and the phys. blends tentatively was attributed to improved charge dissociation and the collection of more favorable energy levels in the blends as a result of partial aggregation of both of the components.

Hit Structure

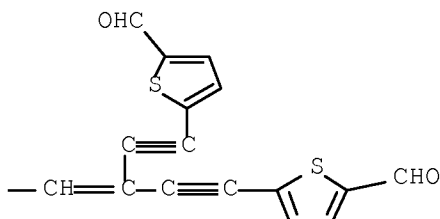
CAS Registry Number
1022991-37-2 CAPLUS

Chemical or Trade Name
2-Thiophenecarboxaldehyde, 5,5'-[2,5-bis(hexyloxy)-1,4-phenylene]bis[2,1-ethynediyl-4,1-phenylene[3-[2-(5-formyl-2-thienyl)ethynyl]-3-buten-1-yn-4,1-diyl]]bis- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)

L3 ANSWER 4 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2008:244421 CAPLUS Full-text

Document Number

148:403337

Title

Triphenylphosphine Incorporation Reactions of Diynyl Complexes Containing a TpRu(NO) Fragment and Isomerization to Ruthenacyclobuta[b]naphthalene

Author/Inventor

Arikawa, Yasuhiro; Asayama, Taiki; Tanaka, Chie; Tashita, Shin-ya; Tsuji, Misako; Ikeda, Kenta; Umakoshi, Keisuke; Onishi, Masayoshi

Patent Assignee/Corporate Source

Department of Applied Chemistry, Faculty of Engineering, Nagasaki University, Nagasaki, 852-8521, Japan

Source

Organometallics (2008), 27(6), 1227-1233 CODEN: ORGND7; ISSN: 0276-7333

Document Type

Journal

Language

English

Abstract

Nitrosylruthenium arylbutadiynyl complexes having a Tp ligand (Tp = BH(pyrazol-1-yl)₃) were prepared, and their reactivities toward PPh₃ incorporation in the presence of HBF₄·Et₂O were described. The PPh₃ incorporation of mono(arylbutadiynyl) complex TpRuCl(C.tpbond.C-C.tpbond.C-C6H4Me)(NO) (1) resulted in the β -phosphonioalkenyl complex (E)-[TpRuCl(CH.C(PPh₃)-C.tpbond.C-C6H4Me)(NO)]BF₄ (2-BF₄), whereas when bis(arylbutadiynyl) TpRu(C.tpbond.C-C.tpbond.C-C6H4Me)₂(NO) (3) was treated, mono- and bis(β -phosphonioalkenyl) complexes (E)-[TpRu(C.tpbond.C-C.tpbond.C-C6H4Me)(CH.C(PPh₃)-C.tpbond.C-C6H4Me)(NO)]BF₄ (4-BF₄) and (E,E)-[TpRu(CH.C(PPh₃)-C.tpbond.C-C6H4Me)₂(NO)](BF₄)₂ [5-(BF₄)₂] were obtained depending on the reaction conditions. On the other hand, an unsym. mixed (arylbutadiynyl)(3-hydroxyalkynyl) complex, TpRu(C.tpbond.C-C.tpbond.C-C6H4Me)[C.tpbond.CCPh₂(OH)](NO) (6), was allowed to react with PPh₃ in the presence of the protic acid to give the α -phosphonioalkenyl [TpRu(C.tpbond.C-C.tpbond.C-C6H4Me)[C(PPh₃)-C.CPh₂(NO)]BF₄ (7-BF₄). Interestingly, thermal isomerization of 7-BF₄ to a ruthena-2-PPh₃-cyclobuta[b]naphthalene [TpRu(CH(PPh₃)[3-Ph-8-(MeC6H4-C.tpbond.C)-C10H4]](NO)]BF₄ (8-BF₄) was observed

Hit Structure

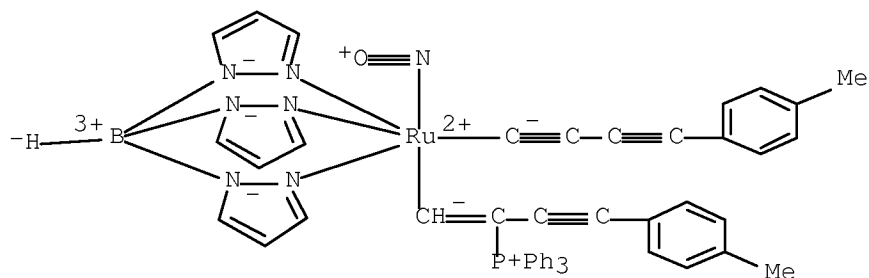
CAS Registry Number
1015477-27-6 CAPLUS

Chemical or Trade Name
Ruthenium(1+), [hydrotris(1H-pyrazolato- κ N1)borato(1-)- κ N2, κ N2', κ N2''] [4-(4-methylphenyl)-1,3-butadiyn-1-

yl] [(1E)-4-(4-methylphenyl)-2-(triphenylphosphonio)-1-buten-3-yn-1-yl]nitrosyl-, (OC-6-24)-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)

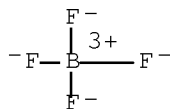
CM 1

CRN 1015477-26-5
 CMF C49 H40 B N7 O P Ru
 CCI CCS



CM 2

CRN 14874-70-5
 CMF B F4
 CCI CCS



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
 (6 CITINGS)

L3 ANSWER 5 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2007:1105260 CAPLUS [Full-text](#)

Document Number

148:11306

Title

Formation and Structural and Dynamic Features of Atropisomeric η^2 -Iminoacyl Zirconium Complexes

Author/Inventor

Spies, Patrick; Kehr, Gerald; Kehr, Seda; Froehlich, Roland; Erker, Gerhard

Patent Assignee/Corporate Source

Organisch-Chemisches Institut, Universitaet Muenster, Muenster, 48149, Germany

Source

Organometallics (2007), 26(23), 5612-5620 CODEN: ORGND7; ISSN: 0276-7333

Document Type

Journal

Language

English

Abstract

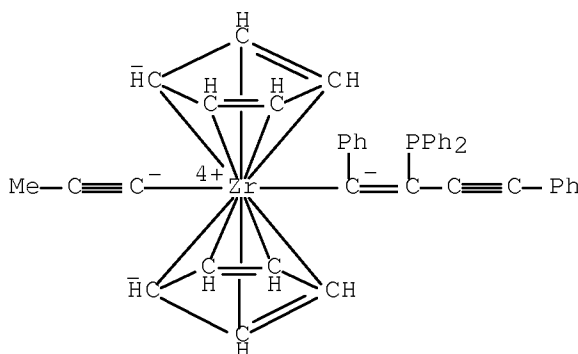
The $\text{Cp}_2\text{ZrCl}[\text{CPh}:\text{C}(\text{PX}_2)\text{C}:\text{tpbond}:\text{CPh}]$ complexes 7a ($\text{X} = \text{Ph}$) and 10 ($\text{X} = \text{C}_6\text{F}_5$) insert tert-butylnitrile into the $\text{Zr}-\text{C}(\text{sp}^2)$ σ bond to yield the iminoacyl zirconocene complexes, $\text{Cp}_2\text{ZrCl}[\text{C}(\text{NCMe}_3)\text{CPh}:\text{C}(\text{PX}_2)\text{C}:\text{tpbond}:\text{CPh}]$ 13a and 13b. X-ray crystal structure anal. of complexes 13a and 13b revealed a chiral atropisomeric structure with a torsion angle of $74.8(2)^\circ$ (13a) and $72.9(6)^\circ$ (13b), resp., around the central iminoacyl/alkenyl $\text{C}(\text{sp}^2)-\text{C}(\text{sp}^2)$ σ bond. In solution an analogous chiral structure is observed. The barrier of interconversion of the enantiomeric atropisomers of 13a and 13b was determined at $\Delta G_{\text{thermod.}}(327\text{K}) = 14.9 \pm 0.3 \text{ kcal mol}^{-1}$ (13a) and $\Delta G_{\text{thermod.}}(325\text{K}) = 14.8 \pm 0.3 \text{ kcal mol}^{-1}$ (13b) by temperature-dependent dynamic NMR spectroscopy. Reaction of 7a and 10 with methyllithium followed by treatment with $\text{B}(\text{C}_6\text{F}_5)_3$ gave the corresponding cationic zirconocene complexes $\text{Cp}_2\text{Zr}^+(\text{THF})[\text{CPh}:\text{C}(\text{PX}_2)\text{C}:\text{tpbond}:\text{CPh}][\text{MeB}(\text{C}_6\text{F}_5)_3]$ 12a and 12b. These complexes took up 2 mol equiv of tert-butylnitrile to yield the cationic N-inside η^2 -iminoacyl zirconocene systems 14a and 14b as isonitrile adducts. The cationic complexes 14a and 14b are also axially chiral. The barriers of enantiomerization ($\Delta G_{\text{thermod.}}(288\text{K}) = 13.1 \pm 0.3 \text{ kcal mol}^{-1}$ (14a), $\Delta G_{\text{thermod.}}(293\text{K}) = 13.4 \pm 0.3 \text{ kcal mol}^{-1}$ (14b)) were also determined by dynamic NMR spectroscopy.

Hit Structure

CAS Registry Number
958635-66-0 CAPLUS

Chemical or Trade Name

Zirconium, bis(η^5 -2,4-cyclopentadien-1-yl) [(1E)-2-(diphenylphosphino)-1,4-diphenyl-1-buten-3-yn-1-yl]-1-propyn-1-yl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L3 ANSWER 6 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2007:995140 CAPLUS [Full-text](#)

Document Number

147:448227

Title

Convenient synthesis of (1-propynyl)arenes through a one-pot double elimination reaction, and their conversion to enynes

Author/Inventor

An, De-Lie; Zhang, Zhiyang; Orita, Akihiro; Mineyama, Hidetaka; Otera, Junzo

Patent Assignee/Corporate Source

Department of Chemistry, College of Chemistry and Chemical Engineering, Hunan University, Changsha, 410082, Peop. Rep. China

Source

Synlett (2007), (12), 1909-1912 CODEN: SYNLES; ISSN: 0936-5214

Document Type

Journal

Language

English

Abstract

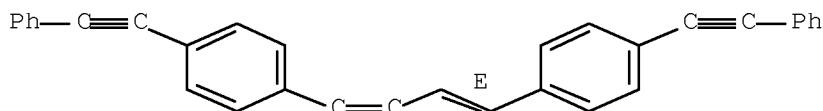
A series of prop-1-ynyl arenes were prepared by one-pot double elimination reaction of EtSO_2Ph , aromatic aldehyde, and $\text{ClPO}(\text{OEt})_2$ in THF with a base such as BuLi and tBuOK . A propargyllithium, which was prepared by treatment of propyn-1-yl arene with BuLi in the presence of 1,3-dimethyl-3,4,5,6-tetrahydro-2(1H)-pyrimidinone (DMPU), reacted with aromatic aldehyde, $\text{ClPO}(\text{OEt})_2$ and tBuOK to afford 4-arylbut-3-en-1-ynyl arene. Photoluminescence of the enynes thus prepared was recorded both in solution and in the solid state.

Hit Structure

CAS Registry Number
951766-78-2 CAPLUS

Chemical or Trade Name

Benzene, 1,1'-(1E)-1-buten-3-yne-1,4-diylbis[4-(2-phenylethynyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

L3 ANSWER 7 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2007:46877 CAPLUS [Full-text](#)

Document Number

148:284829

Title

Synthesis of smallest unit model of graphite intercalation compound and its possibility

Author/Inventor

Ogoshi, Sensuske

Patent Assignee/Corporate Source

Department of Applied Chemistry, Faculty of Engineering, Osaka University, Japan

Source

Asahi Garasu Zaidan Josei Kenkyu Seika Hokoku (2006) 01.03.07/1-01.03.07/8 CODEN: AGSHEN; ISSN: 0919-9179

Document Type

Journal; (computer optical disk)

Language

Japanese

Abstract

Graphite is perhaps the simplest layered structure. Many substances can be intercalated between layers of graphite. Upon intercalation, the graphite layers moved apart somewhat due to the intercalated atom. However, the layers still keep parallel each other which would be the key for the formation of intercalation compds. Thus, compds. having two aromatic rings, which can change the distance between the rings and keep parallel to each other, were designed and synthesized. The target compound was 1,8-bis[6-(1-naphthalenyl)-3-hexene-1,5-diynyl]anthracene.

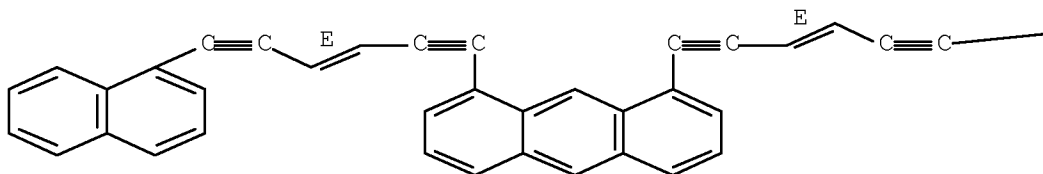
Hit Structure

CAS Registry Number
1007602-95-0 CAPLUS

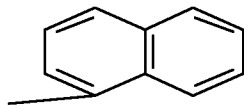
Chemical or Trade Name

Anthracene, 1,8-bis[(3E)-6-(1-naphthalenyl)-3-hexene-1,5-diyn-1-yl]- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L3 ANSWER 8 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2006:82014 CAPLUS [Full-text](#)

Document Number

144:334159

Title

Light harvesting tetrafullerene nanoarray for organic solar cells

Author/Inventor

Atienza, Carmen M.; Fernandez, Gustavo; Sanchez, Luis; Martin, Nazario; Dantas, Ines Sa; Wienk, Martijn M.; Janssen, Rene A. J.; Rahman, G. M. Aminur; Guld, Dirk M.

Patent Assignee/Corporate Source

Departamento de Quimica Organica, Facultad de Ciencias Quimicas, Universidad Complutense, Madrid, E-28040, Spain

Source

Chemical Communications (Cambridge, United Kingdom) (2006), (5), 514-516 CODEN: CHCOFS; ISSN: 1359-7345

Document Type

Journal

Language

English

Abstract

A light absorbing π -conjugated oligomer-tetrafullerene nanoarray was synthesized and its photophys. study reveals an intramol. energy transfer. A photovoltaic device fabricated from this nanoarray and poly(3-hexylthiophene) shows an external quantum efficiency of 15% at 500 nm.

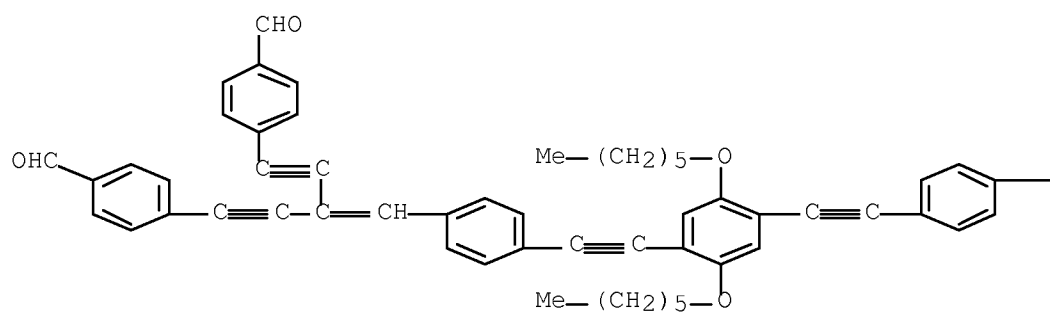
Hit Structure

CAS Registry Number
880486-74-8 CAPLUS

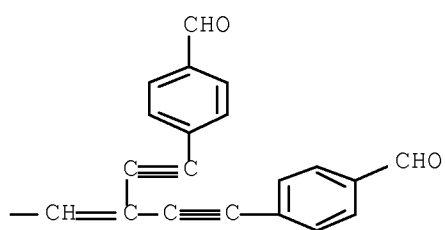
Chemical or Trade Name

Benzaldehyde, 4,4'-[[2,5-bis(hexyloxy)-1,4-phenylene]bis[2,1-ethynediyl]-4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis-(9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS
RECORD (20 CITINGS)

Accession Number

2005:1004691 CAPLUS [Full-text](#)

Document Number

143:306181

Title

Process for preparation of π -conjugated aromatic ring-containing acetylene derivatives as organic electroluminescent devices

Author/Inventor

Sato, Fumie; Takayama, Yuuki

Patent Assignee/Corporate Source

Nissan Chemical Industries, Ltd., Japan

Source

PCT Int. Appl., 82 pp. CODEN: PIXXD2

Document Type

Patent

Language

Japanese

Patent Information

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005085176	A1	20050915	WO 2005-JP3950	20050308
US 20070176164	A1	20070802	US 2007-591950	20070307

Abstract

This invention pertains to a method for producing π -conjugated aromatic ring-containing acetylene derivs. via coupling reaction in the presence of palladium and Cu(I) catalysts. For example, the compound I was prepared in a multi-step synthesis in good yield. The title compds. are useful as electroluminescent devices.

Hit Structure

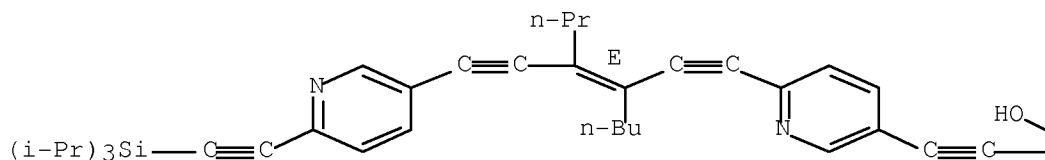
CAS Registry Number

740810-64-4 CAPLUS

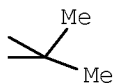
Chemical or Trade Name

3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



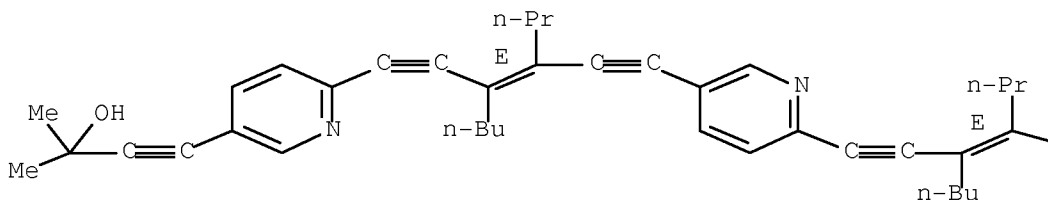
CAS Registry Number

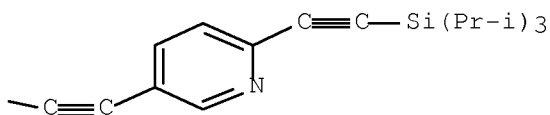
740810-65-5 CAPLUS

Chemical or Trade Name

3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

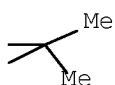
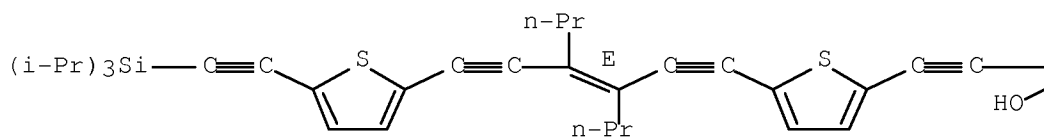
PAGE 1-A





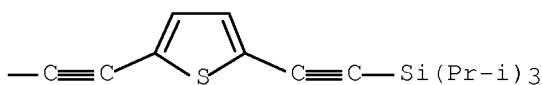
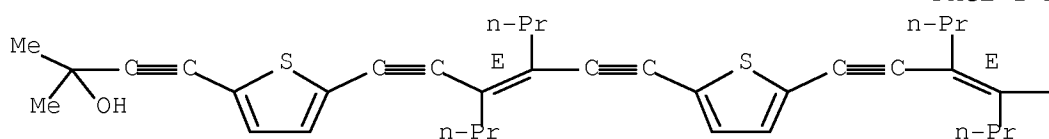
CAS Registry Number
740810-67-7 CAPLUS

Chemical or Trade Name
3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)



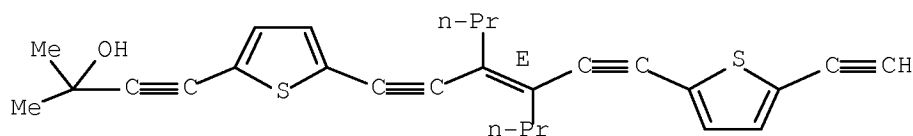
CAS Registry Number
740810-68-8 CAPLUS

Chemical or Trade Name
3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)



CAS Registry Number
864683-96-5 CAPLUS

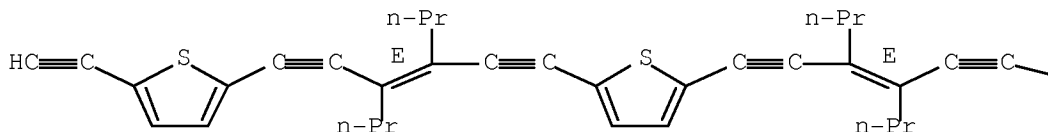
Chemical or Trade Name
3-Butyn-2-ol, 4-[5-[(3E)-5-ethyl-4-[2-(5-ethynyl-2-thienyl)ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)



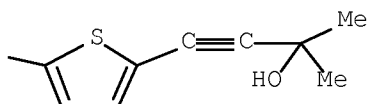
CAS Registry Number
864683-97-6 CAPLUS

Chemical or Trade Name
3-Butyn-2-ol, 4-[5-[(3E)-4-[2-(5-ethynyl-2-thienyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl-2-methyl- (CA INDEX NAME)

PAGE 1-A

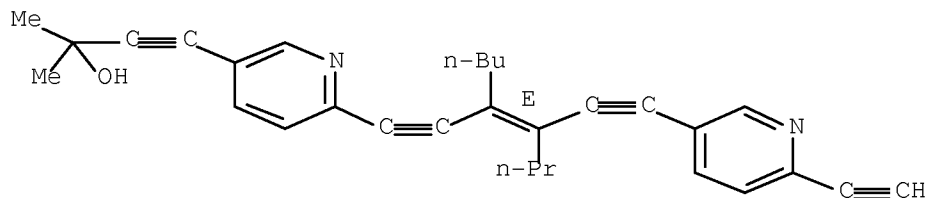


PAGE 1-B



CAS Registry Number
864684-01-5 CAPLUS

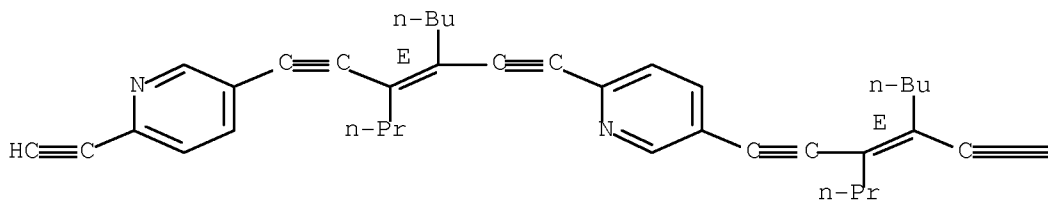
Chemical or Trade Name
3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)



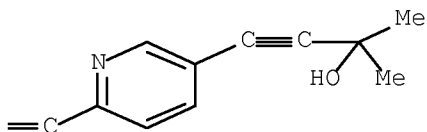
CAS Registry Number
864684-02-6 CAPLUS

Chemical or Trade Name
3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-(6-ethynyl-3-pyridinyl)ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

PAGE 1-A



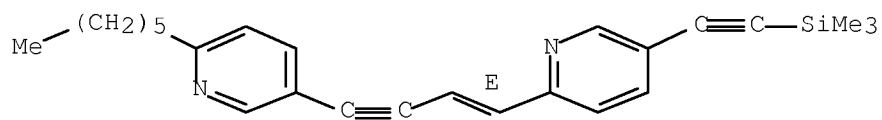
PAGE 1-B



CAS Registry Number

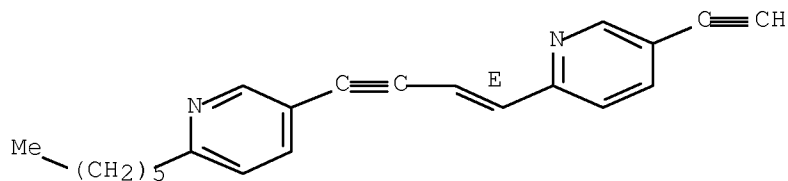
864684-11-7 CAPLUS

Chemical or Trade Name
Pyridine, 2-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)



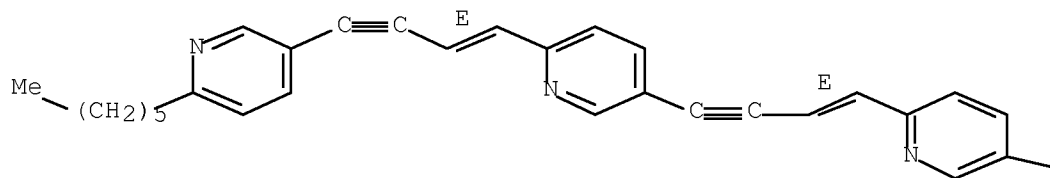
CAS Registry Number
864684-12-8 CAPLUS

Chemical or Trade Name
Pyridine, 5-ethynyl-2-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



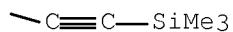
CAS Registry Number
864684-13-9 CAPLUS

Chemical or Trade Name
Pyridine, 2-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-5-[(3E)-4-[5-[2-(trimethylsilyl)ethynyl]-2-pyridinyl]-3-buten-1-yn-1-yl]- (CA INDEX NAME)



PAGE 1-A

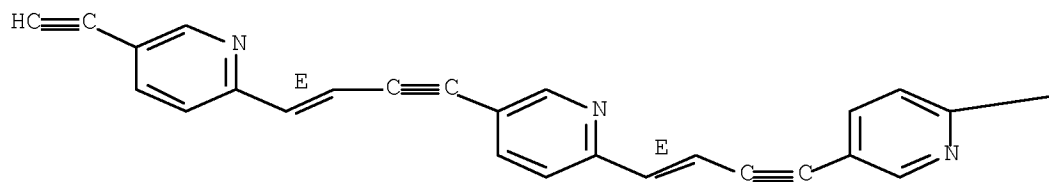
PAGE 1-B



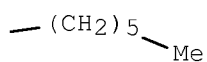
CAS Registry Number
864684-15-1 CAPLUS

Chemical or Trade Name
Pyridine, 5-ethynyl-2-[(1E)-4-[6-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]- (CA INDEX NAME)

PAGE 1-A

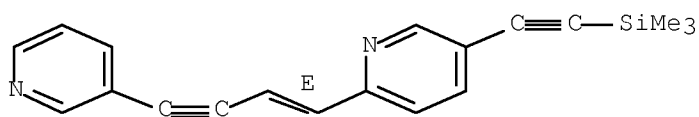


PAGE 1-B



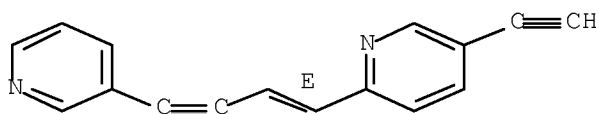
CAS Registry Number
864684-18-4 CAPLUS

Chemical or Trade Name
Pyridine, 2-[(1E)-4-(3-pyridinyl)-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)



CAS Registry Number
864684-19-5 CAPLUS

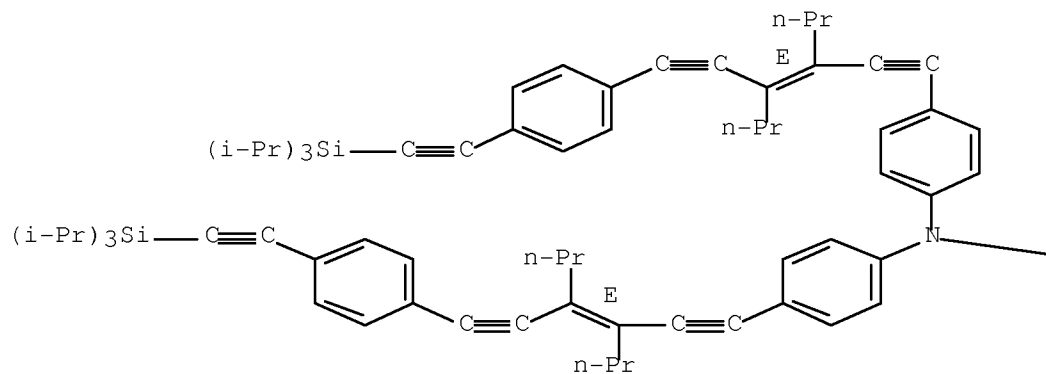
Chemical or Trade Name
Pyridine, 5-ethynyl-2-[(1E)-4-(3-pyridinyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



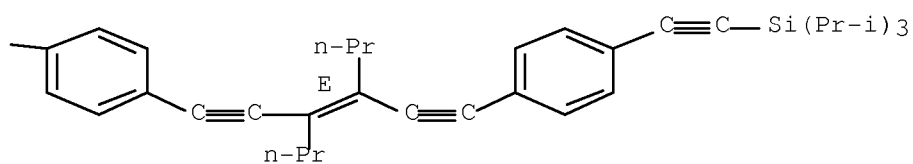
CAS Registry Number
864684-31-1 CAPLUS

Chemical or Trade Name
Benzeneamine, N-[4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]phenyl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]-N-[4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

PAGE 1-A



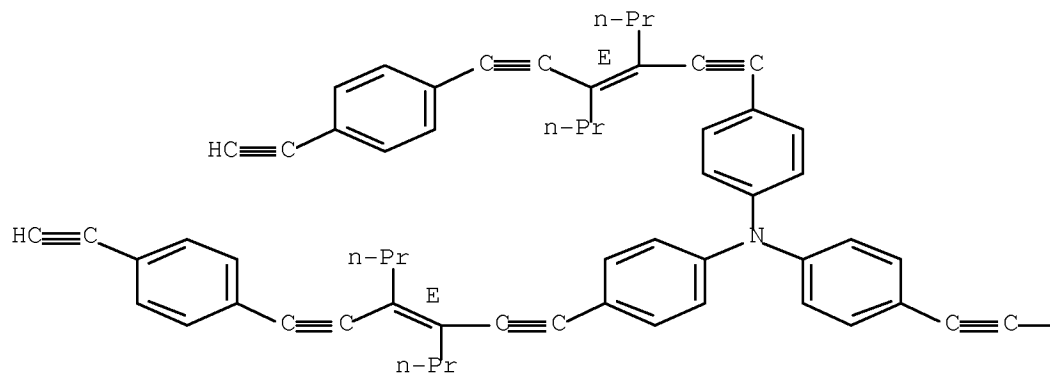
PAGE 1-B



CAS Registry Number
864694-32-2 CAPLUS

Chemical or Trade Name
Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-(4-ethynylphenyl)ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

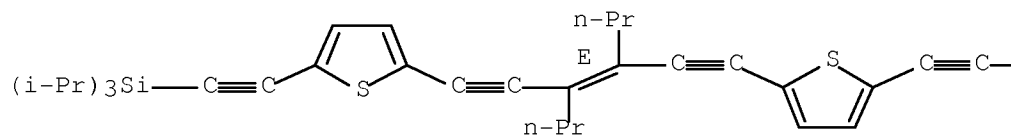
PAGE 1-A



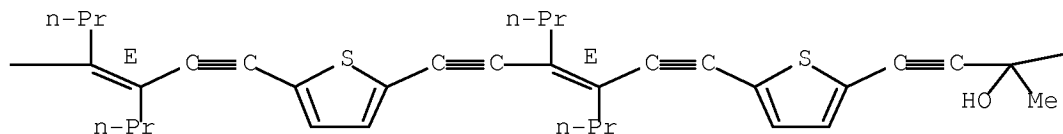
Chemical or Trade Name
3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

Chemical or Trade Name
3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



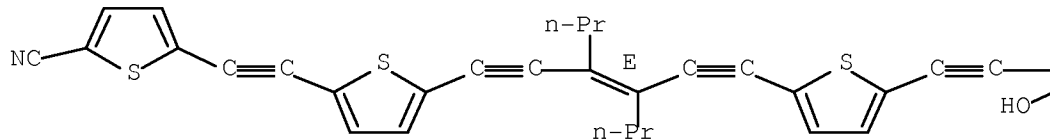
PAGE 1-C



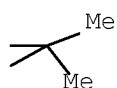
CAS Registry Number
864684-03-7 CAPLUS

Chemical or Trade Name
2-Thiophenecarbonitrile, 5-[2-[5-[(3E)-5-ethyl-4-[2-[5-(3-hydroxy-3-methyl-1-butyn-1-yl)-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]- (CA INDEX NAME)

PAGE 1-A

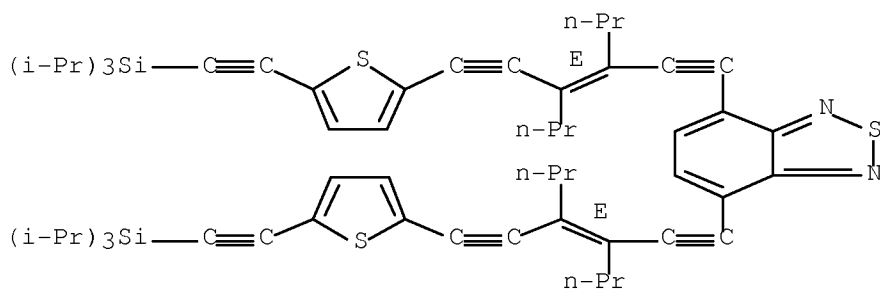


PAGE 1-B



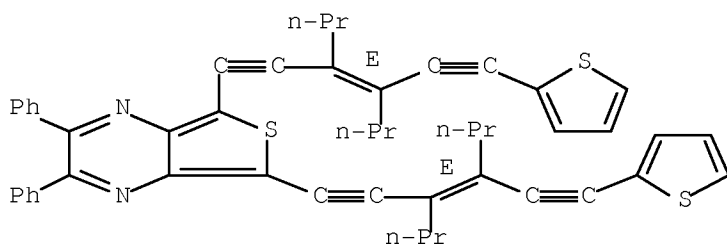
CAS Registry Number
864684-06-0 CAPLUS

Chemical or Trade Name
2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)



CAS Registry Number
864684-09-3 CAPLUS

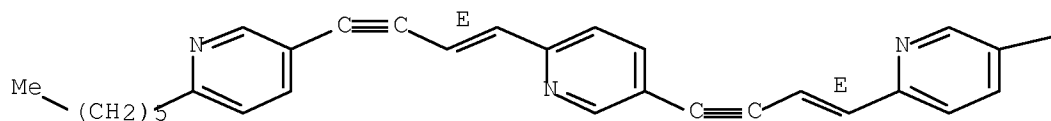
Chemical or Trade Name
Thieno[3,4-b]pyrazine, 5-[(3E)-3,4-dipropyl-6-(2-thienyl)-3-hexene-1,5-diyn-1-yl]-2,3-diphenyl-7-[(3E)-3-propyl-4-[2-(2-thienyl)ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)



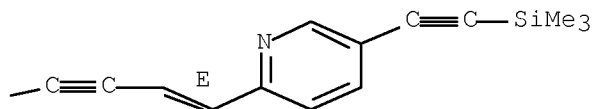
CAS Registry Number
864684-16-2 CAPLUS

Chemical or Trade Name
Pyridine, 2-[(1E)-4-[6-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

PAGE 1-A

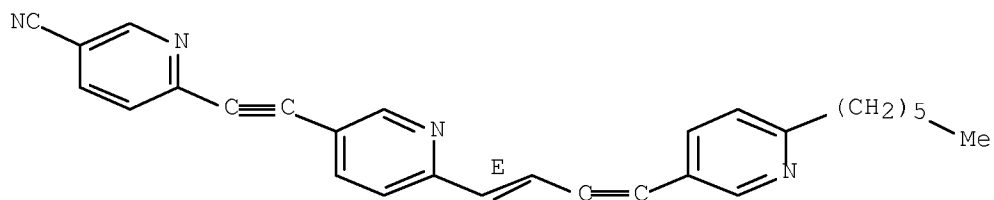


PAGE 1-B



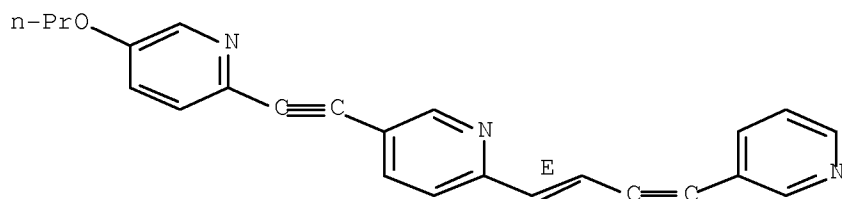
CAS Registry Number
864684-17-3 CAPLUS

Chemical or Trade Name
3-Pyridinecarbonitrile, 6-[2-[6-[(1E)-4-(6-hexyl-3-pyridinyl)-1-buten-3-yn-1-yl]-3-pyridinyl]ethynyl]- (CA INDEX NAME)



CAS Registry Number
864684-20-8 CAPLUS

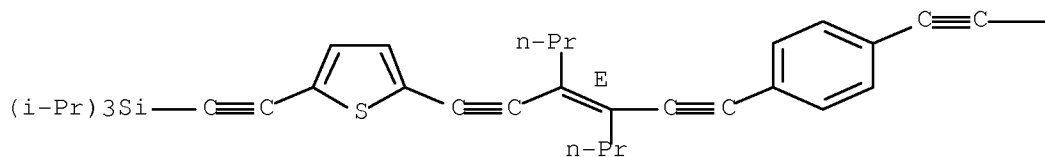
Chemical or Trade Name
Pyridine, 5-[2-(5-propoxy-2-pyridinyl)ethynyl]-2-[(1E)-4-(3-pyridinyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



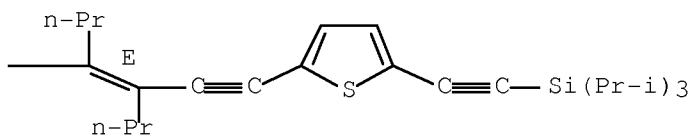
CAS Registry Number
864684-21-9 CAPLUS

Chemical or Trade Name
Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[(3E)-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[2-[tris(1-methylethyl)silyl]ethynyl]- (CA INDEX NAME)

PAGE 1-A



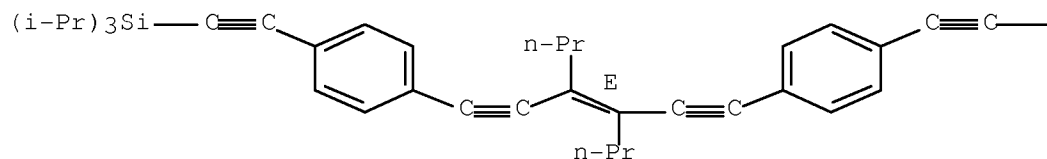
PAGE 1-B



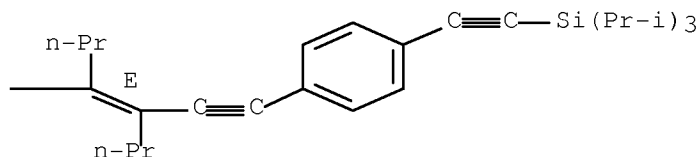
CAS Registry Number
864684-22-0 CAPLUS

Chemical or Trade Name
Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

PAGE 1-A



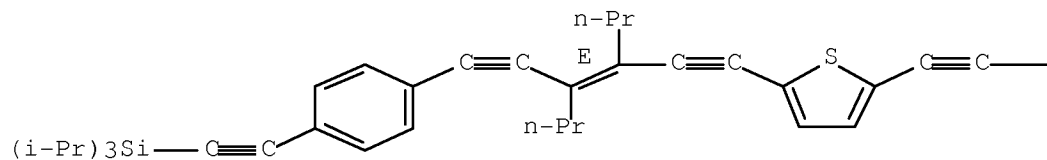
PAGE 1-B



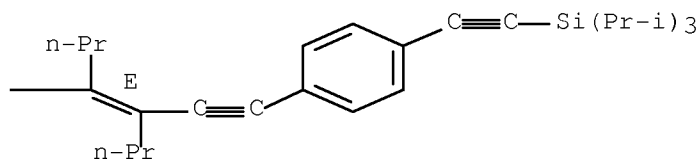
CAS Registry Number
864684-23-1 CAPLUS

Chemical or Trade Name
Thiophene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

PAGE 1-A



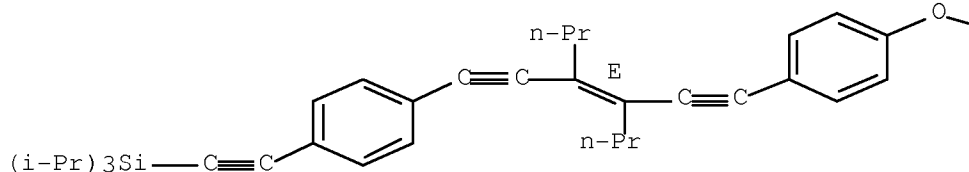
PAGE 1-B



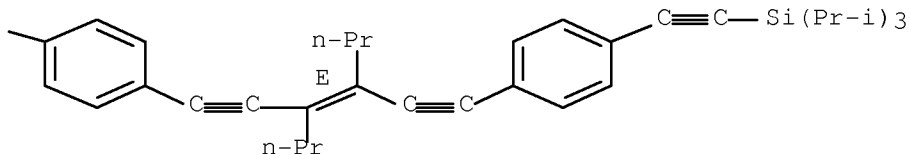
CAS Registry Number
864684-24-2 CAPLUS

Chemical or Trade Name
Silane, [oxybis[4,1-phenylene[(3E)-3,4-dipropyl-3-hexene-1,5-diyne-6,1-diyl]-4,1-phenylene-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



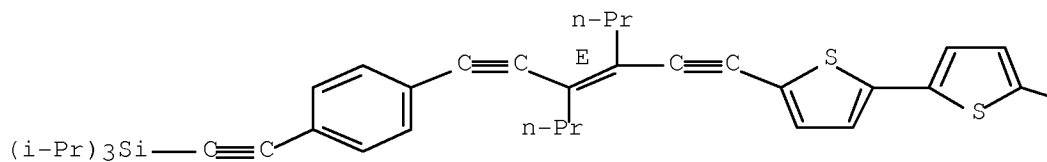
PAGE 1-B



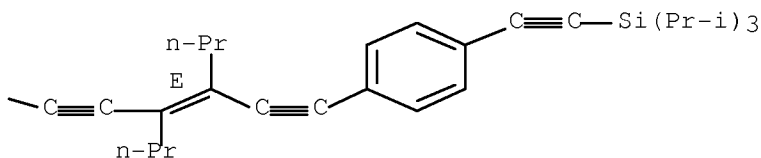
CAS Registry Number
864684-25-3 CAPLUS

Chemical or Trade Name
2,2'-Bithiophene, 5-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-5'-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

PAGE 1-A



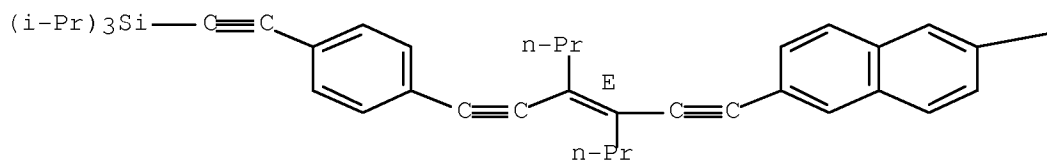
PAGE 1-B

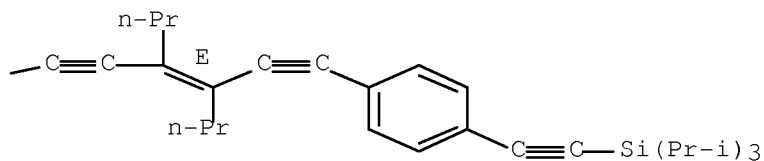


CAS Registry Number
864684-26-4 CAPLUS

Chemical or Trade Name
Naphthalene, 2-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

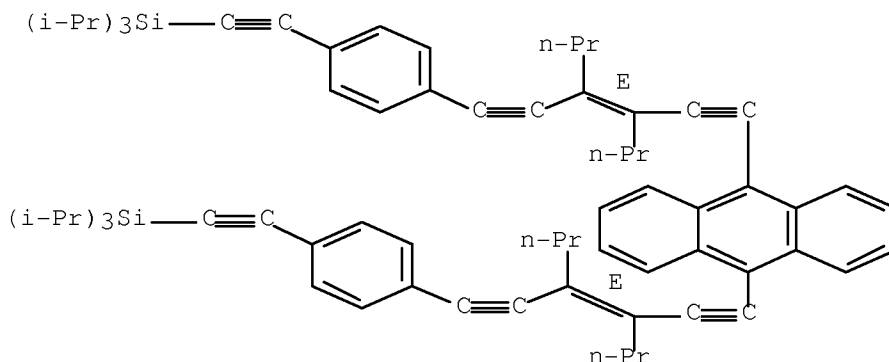
PAGE 1-A





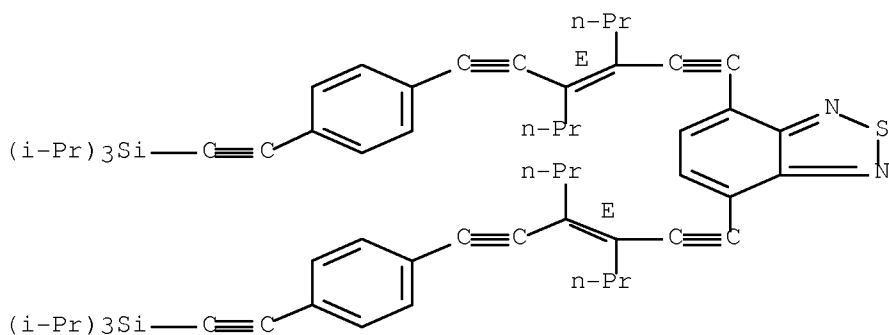
CAS Registry Number
864684-27-5 CAPLUS

Chemical or Trade Name
Anthracene, 9-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-10-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)



CAS Registry Number
864684-28-6 CAPLUS

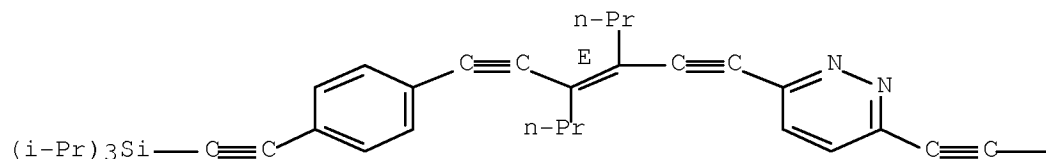
Chemical or Trade Name
2,1,3-Benzothiadiazole, 4-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-7-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)



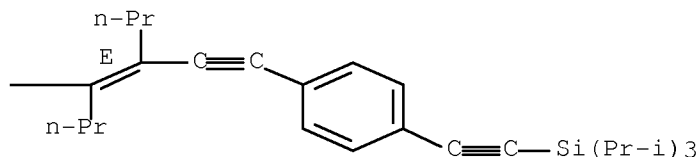
CAS Registry Number
864684-29-7 CAPLUS

Chemical or Trade Name
Pyridazine, 3-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-6-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

PAGE 1-A



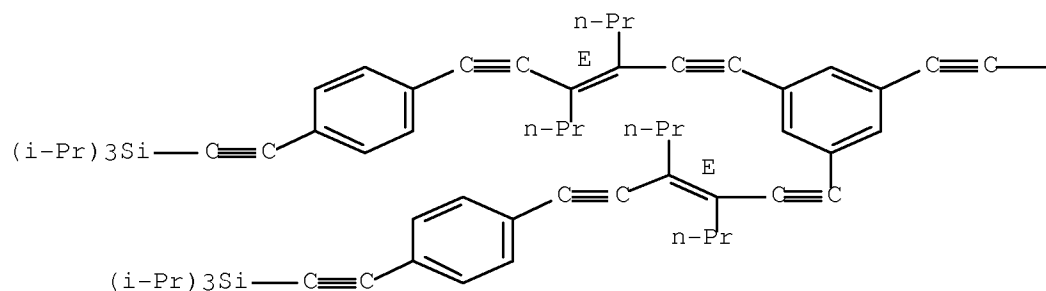
PAGE 1-B



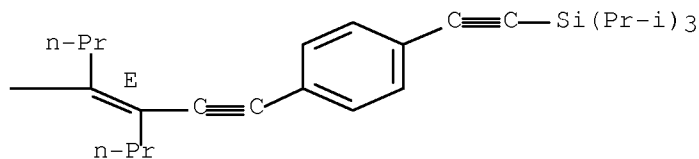
CAS Registry Number
864684-30-0 CAPLUS

Chemical or Trade Name
Benzene, 1-[(3E)-3,4-dipropyl-6-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diyn-1-yl]-3-[(3E)-5-ethyl-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-penten-1-yn-1-yl]-5-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]- (CA INDEX NAME)

PAGE 1-A

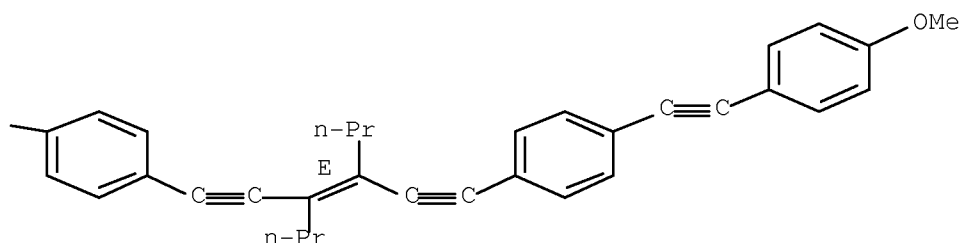
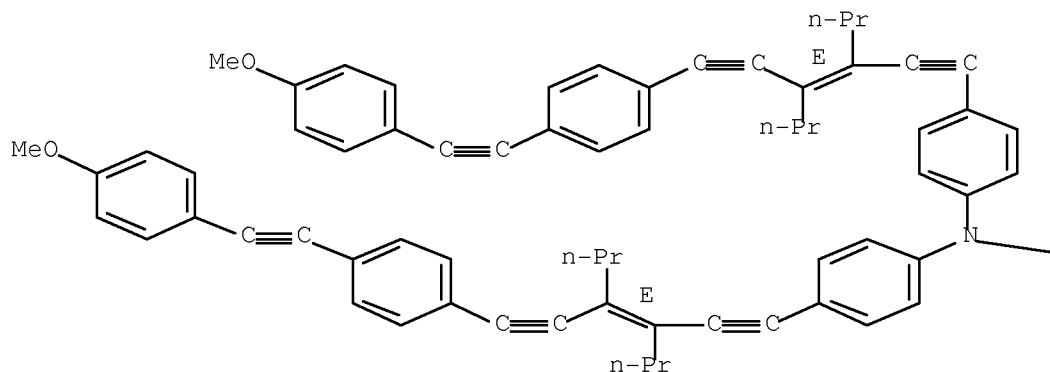


PAGE 1-B



CAS Registry Number
864684-33-3 CAPLUS

Chemical or Trade Name
Benzenamine, N-[4-[(3E)-5-ethyl-4-[2-[4-[2-[4-(methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]phenyl]-4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-N-[4-[(3E)-4-[2-[4-[2-(4-methoxyphenyl)ethynyl]phenyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)



L3 ANSWER 10 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2005:354187 CAPLUS [Full Text](#)

Document Number

143:333

Title

Cytotoxicities, cell cycle and caspase evaluations of 1,6-diaryl-3(Z)-hexen-1,5-diyne, 2-(6-aryl-3(Z)-hexen-1,5-diynyl)anilines and their derivatives

Author/Inventor

Lin, Chi-Fong; Lo, Yu-Hsiang; Hsieh, Ming-Chu; Chen, Yi-Hua; Wang, Jeh-Jeng; Wu, Ming-Jung

Patent Assignee/Corporate Source

School of Chemistry, Kaohsiung Medical University, Kaohsiung, Taiwan

Source

Bioorganic & Medicinal Chemistry (2005), 13(10), 3565-3575 CODEN: BMECEP; ISSN: 0968-0896

Document Type

Journal

Language

English

Abstract

A series of compds. showed growth inhibition effects on a full panel of 60 human cancer cell lines, and most of the average IC50 values of the indicated analogs were from <0.01 to 96.6 μ M, in which a 2-thienyl analog and the thioanisole analog revealed the highest cytotoxic activity with the cancer cell lines at 10⁻⁷M concentration range. During the cell cycle anal., a moderate to high apoptotic progress induction was shown by several compared with the control, which 2-(6-(2-thienyl)-3(Z)-hexen-1,5-diynyl)aniline (I) showed the highest apoptotic effect. I and the thioanisole analog displayed a significant G2/M phase arrest in the cell growth cycle compared with other derivs., which the proportions of the G2/M phase cells were accumulated to 71.5% and 82.6%, resp. Moreover, the colorimetric assay of the I and the thioanisole analog also provided advanced evidence to the relationship between the compds. and the caspase-3 enzyme, which was one of the major promoters of apoptotic effect.

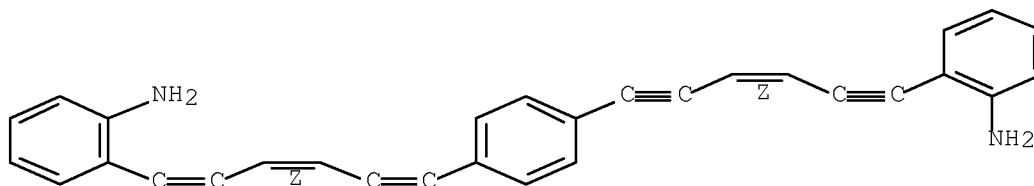
Hit Structure

CAS Registry Number

852619-13-7 CAPLUS

Chemical or Trade Name

Benzenamine, 2,2'-[1,4-phenylenedi-(3Z)-3-hexene-1,5-diyne-6,1-diyl]bis-(9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)

L3 ANSWER 11 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2004:832644 CAPLUS [Full-text](#)

Document Number

142:38113

Title

Site-Selective Monofunctionation of Dialkynylpyridines and Its Application for Preparation of Highly Fluorescent π -Conjugated Oligomers

Author/Inventor

Takayama, Yuuki; Hanazawa, Takeshi; Andou, Tomohiro; Muraoka, Kenji; Ohtani, Hiroyuki; Takahashi, Mizuki; Sato, Fumie

Patent Assignee/Corporate Source

Department of Biomolecular Engineering, Tokyo Institute of Technology, Midori-ku, Yokohama, Kanagawa, 226-8501, Japan

Source

Organic Letters (2004), 6(23), 4253-4256 CODEN: ORLEF7; ISSN: 1523-7060

Document Type

Journal

Language

English

Abstract

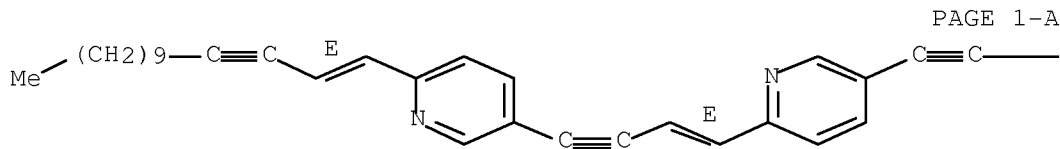
Reaction of Ti(O-*i*-Pr)₄/2-*i*-PrMgCl reagent with 2,*n*-bis(trimethylsilyl)ethynylpyridines, where *n* is 3, 4, 5, and 6, or with 3,4-bis(trimethylsilyl)ethynylpyridines, proceeded with excellent site-selectivity to afford the corresponding monofunctionated complex. Synthetic application of the reaction was demonstrated by an efficient preparation of π -conjugated oligomers having pyridine and enyne units alternately, which possess intense blue fluorescence emission. Thus, reaction of 2,3-bis(trimethylsilyl)ethynylpyridine with Ti(O-*i*-Pr)₄/2-*i*-PrMgCl reagent in Et₂O gave 84% (Z)-2-[2-(trimethylsilyl)ethynyl]-3-[(trimethylsilyl)ethynyl]pyridine.

Hit Structure

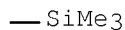
CAS Registry Number
805240-17-9 CAPLUS

Chemical or Trade Name

Pyridine, 2-[(1E)-4-[6-[(1E)-1-tetradecen-3-yn-1-yl-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)



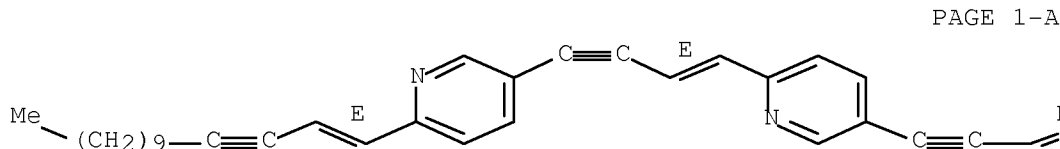
PAGE 1-B



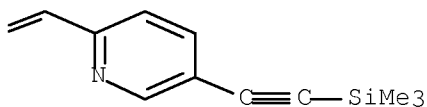
CAS Registry Number
805240-18-0 CAPLUS

Chemical or Trade Name

Pyridine, 2-[(1E)-4-[6-[(1E)-4-[6-[(1E)-1-tetradecen-3-yn-1-yl-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

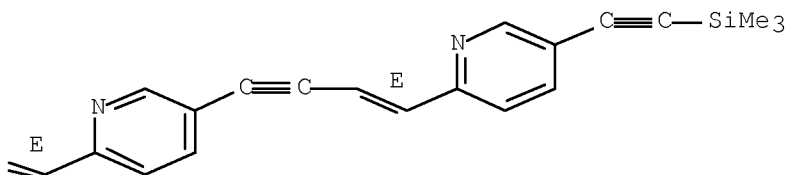
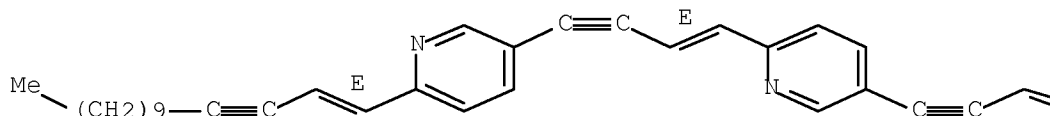


PAGE 1-A



CAS Registry Number
805240-19-1 CAPLUS

Chemical or Trade Name
Pyridine, 2-[(1E)-4-[6-[(1E)-4-[6-(1E)-1-tetradecen-3-yn-1-yl-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L3 ANSWER 12 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2004:566840 CAPLUS [Full-text](#)

Document Number

141:261152

Title

π -Conjugated Dendrimers Based on Bis(enediynyl)benzene Units

Author/Inventor

Hwang, Gil Tae; Kim, Byeang Hyeon

Patent Assignee/Corporate Source

National Research Laboratory, Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

Source

Organic Letters (2004), 6(16), 2669-2672 CODEN: ORLEF7; ISSN: 1523-7060

Document Type

Journal

Language

English

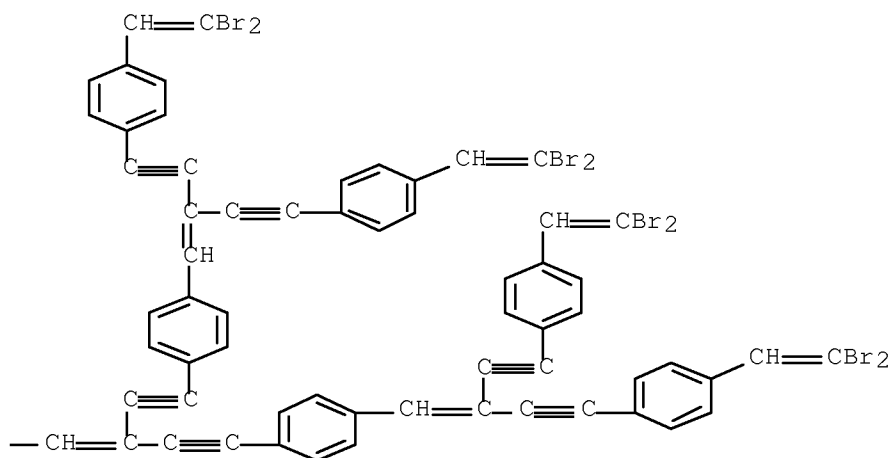
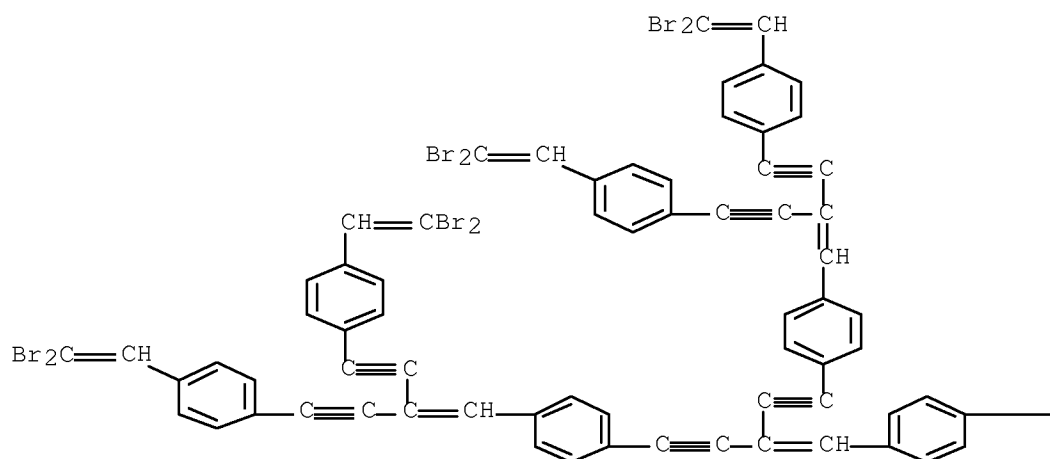
Abstract

We have synthesized a new family of π -conjugated dendrimers that are based on bis(enediynyl)benzene units by using both divergent and convergent approaches. The compds. at all three generations have strong bluish-green fluorescence, especially the third-generation dendrimer, which has the highest extinction coefficient and quantum efficiency in this series.

Hit Structure

CAS Registry Number
754233-16-4 CAPLUS

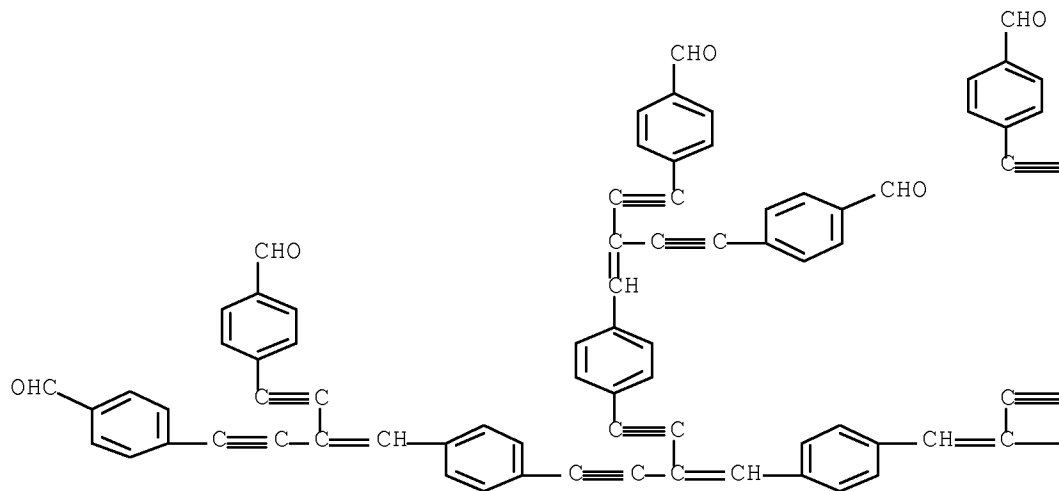
Chemical or Trade Name
Benzene, 1,4-bis[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]-9CI (CA INDEX NAME)



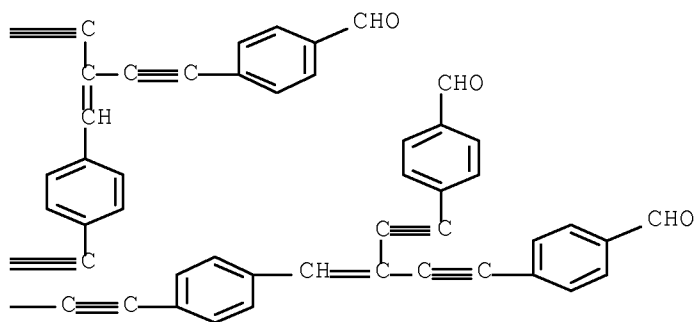
CAS Registry Number
754233-18-6 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-bis[[3-[[4-[[4-[[4-(4-formylphenyl)-2-[[4-(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-(4-(4-formylphenyl)-2-[[4-(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[[4-(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)

PAGE 1-A

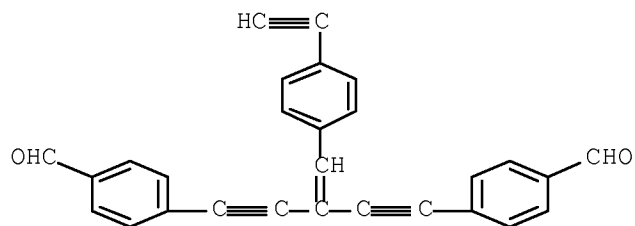


PAGE 1-B



CAS Registry Number
206191-75-1 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS
RECORD (17 CITINGS)

Accession Number

2004:480115 CAPLUS [Full-text](#)

Document Number

141:190674

Title

Synthesis of Conjugated Oligomers Having Aromatic and Enediyne Units Alternately in the Backbone that Show Intense Fluorescence Emission

Author/Inventor

Nakano, Yuuki; Ishizuka, Kenichi; Muraoka, Kenji; Ohtani, Hiroyuki; Takayama, Yuuki; Sato, Fumie

Patent Assignee/Corporate Source

Department of Biomolecular Engineering, Tokyo Institute of Technology, Midori, Yokohama, Kanagawa, 226-8501, Japan

Source

Organic Letters (2004), 6(14), 2373-2376 CODEN: ORLEF7; ISSN: 1523-7060

Document Type

Journal

Language

English

Abstract

Synthesis and fluorescence properties of *n*-conjugated compds. I (*n* = 1 - 3; X = 1,4-phenylene, 2,5-pyridine, 2,5-thiophene; R = *n*-Pr, *n*-Bu) having alternately an aromatic or heteroarom. ring and an enediyne unit in the backbone are described.

Hit Structure

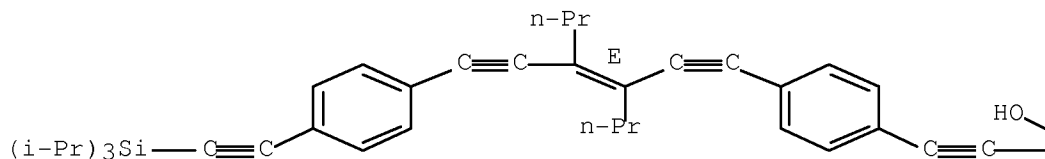
CAS Registry Number

740810-61-1 CAPLUS

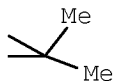
Chemical or Trade Name

3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



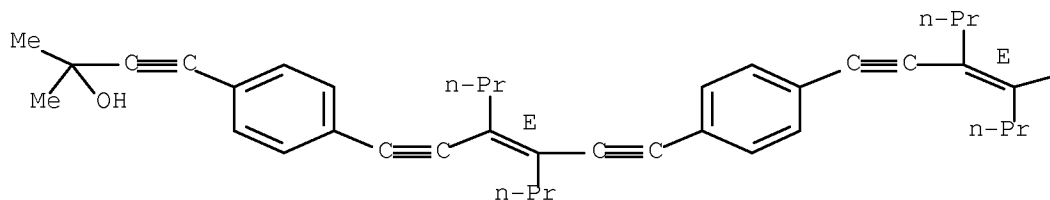
CAS Registry Number

740810-62-2 CAPLUS

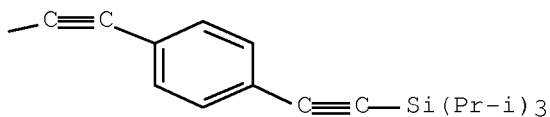
Chemical or Trade Name

3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[4-[[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

PAGE 1-A



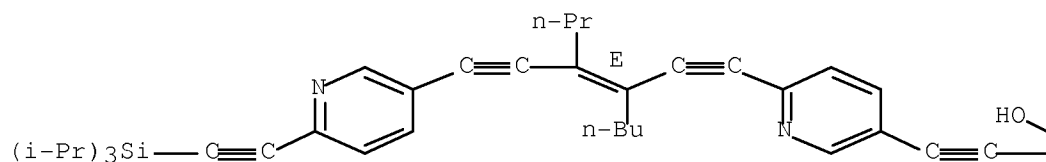
PAGE 1-B



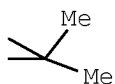
CAS Registry Number
740810-64-4 CAPLUS

Chemical or Trade Name
3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

PAGE 1-A



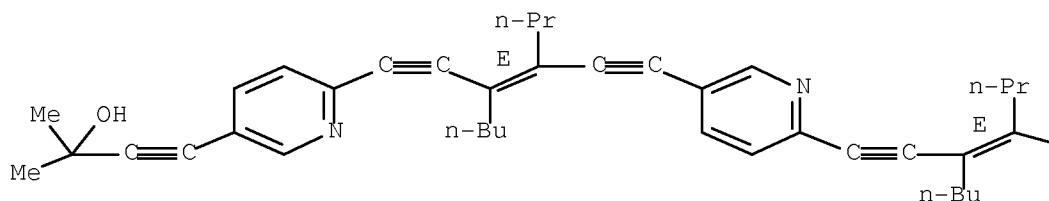
PAGE 1-B



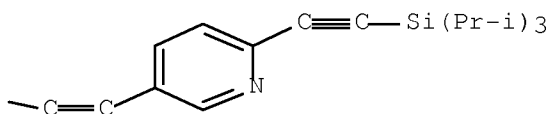
CAS Registry Number
740810-65-5 CAPLUS

Chemical or Trade Name
3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

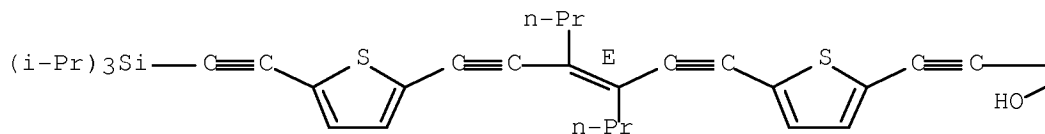


CAS Registry Number

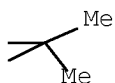
740810-67-7 CAPLUS

Chemical or Trade Name
3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

PAGE 1-A



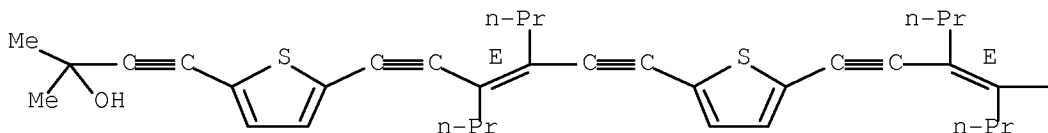
PAGE 1-B



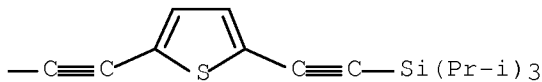
CAS Registry Number
740810-68-8 CAPLUS

Chemical or Trade Name
3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

PAGE 1-A



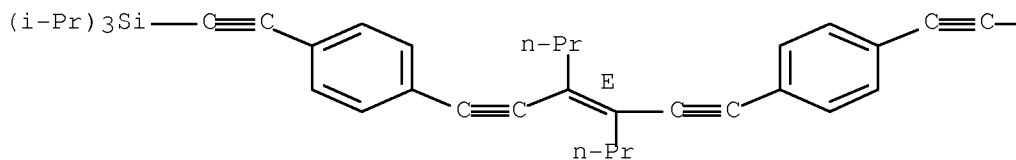
PAGE 1-B



CAS Registry Number
740810-63-3 CAPLUS

Chemical or Trade Name
3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[[4-[(3E)-3-propyl-4-[[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

PAGE 1-A



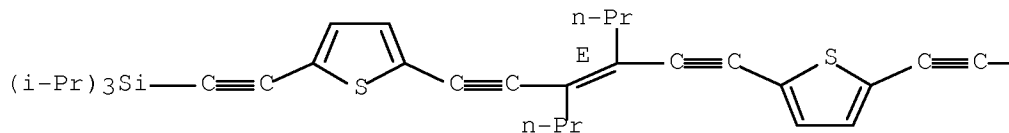
CCCCC=C(CCCC)C#Cc1ccc(cc1)C#CC(CCCC)=C(CCCC)C#Cc2ccc(cc2)C#CC(C)(O)CCCC
$$\begin{array}{c} \text{Me} \\ \diagup \\ \text{Me} \end{array}$$

Chemical or Trade Name
3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[tris[1-methylethyl]silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-2-methyl- (CA INDEX NAME)

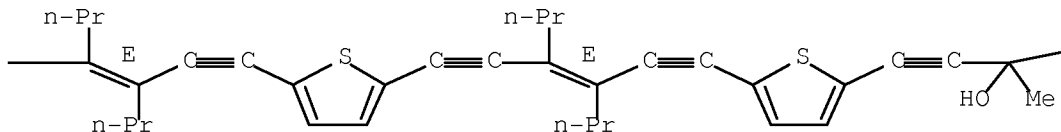
$$(i\text{-Pr})_3\text{Si}-\text{C}\equiv\text{C}-\text{C}_6\text{H}_4-\text{C}\equiv\text{C}-\text{C}(\text{n-Pr})=\text{C}(\text{n-Bu})-\text{C}\equiv\text{C}-\text{C}_6\text{H}_4-\text{C}\equiv\text{C}-\text{C}\equiv\text{C}-\text{C}_6\text{H}_4-\text{C}\equiv\text{C}-\text{Si}(i\text{-Pr})_3$$
CCCCC=C(CCCC)C#Cc1cccnc1C#CC(CCCC)=C(CCCC)C#Cc2cccnc2C#CC(C)(C)O
CC(C)C(C)C

Chemical or Trade Name
3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethynyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



PAGE 1-C



OS.CITING REF COUNT: 23 THERE ARE 23 CAPLUS RECORDS THAT CITE THIS RECORD (24 CITINGS)

L3 ANSWER 14 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2004:382959 CAPLUS [Full-text](#)

Document Number

141:88772

Title

Electrochemical and theoretical study of a family of fully conjugated dendritic oligomers

Author/Inventor

Osorio, Gabriela; Frontana, Carlos; Guadarrama, Patricia; Frontana-Urbe, Bernardo A.

Patent Assignee/Corporate Source

Instituto de Química, UNAM, Circuito Exterior Ciudad Universitaria, Mexico, 04510, Mex.

Source

Journal of Physical Organic Chemistry (2004), 17(5), 439-447 CODEN: JPOCEE; ISSN: 0894-3230

Document Type

Journal

Language

English

Abstract

Novel dendritic oligomers of β,β -dibromo-4-ethynylstyrene and formyl-4-ethynylstyrene were electrochem. and theor. studied to gain a better insight into their redox behavior. Correlations between calculated ionization and exptl. oxidation potentials (anodic peak potentials) were established. The best correlation was obtained when two important effects are considered in the theor. calcs., probing their strong influence: (a) structural re- accommodation in the formed radical cation and (b) solvation effects. The effect of dendritic terminal groups (dibromovinyl and formyl groups) was also analyzed. A different redox behavior was observed for these two terminal groups, presumably due to a difference in their oxidation mechanisms. A global chemical transformation for the oxidation of dibromovinyl-terminated oligomers was proposed, providing a satisfactory explanation of the electrochem. behavior within this family of (presence of adsorptive phenomena). Taking these results into account, it is possible to explain how the cation-radical species formed in these conjugated dendritic oligomers behave when cyclic voltammetry technique is applied.

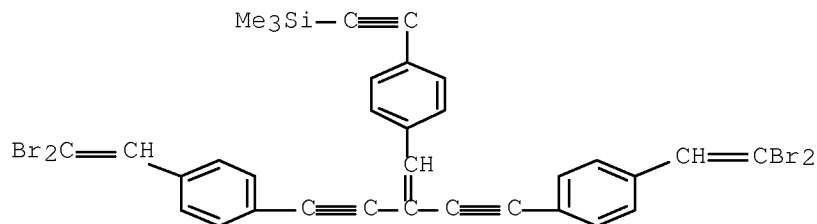
Hit Structure

CAS Registry Number

716327-89-8 CAPLUS

Chemical or Trade Name

Silane, [[4-[4-[4-(2,2-dibromoethenyl)phenyl]phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-, radical ion(1+) (9CI) (CA INDEX NAME)



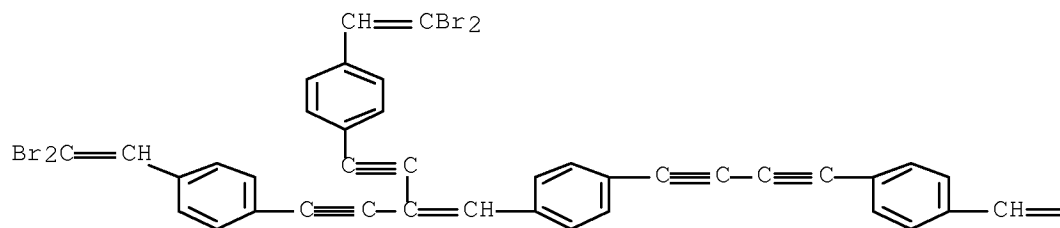
CAS Registry Number

716327-90-1 CAPLUS

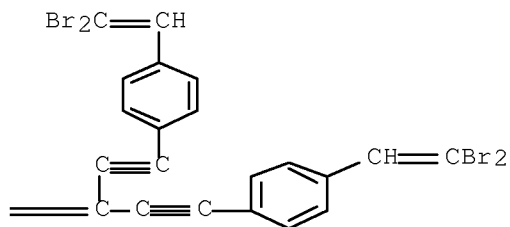
Chemical or Trade Name

Benzene, 1,1'-(1,3-butadiene-1,4-diyl)bis[4-[4-[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]-, radical ion(1+) (9CI) (CA INDEX NAME)

PAGE 1-A



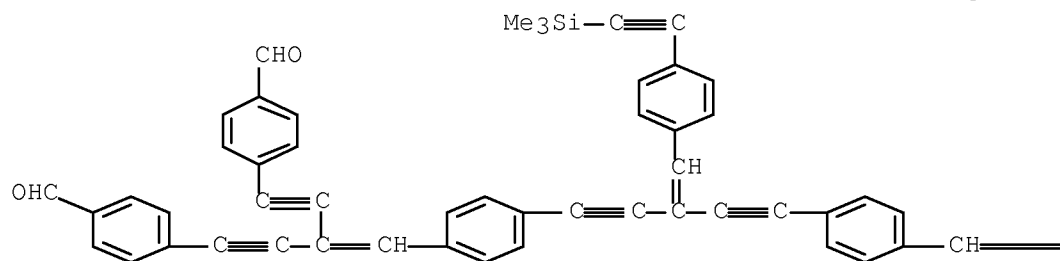
PAGE 1-B



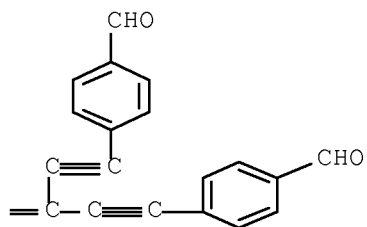
CAS Registry Number
716327-91-2 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[[3-[[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]]bis[4,1-phenylene[3-[[4-formylphenyl]ethynyl]-3-buten-1-yne-4,1-diyl]]]bis-, radical ion(1+) (9CI) (CA INDEX NAME)

PAGE 1-A

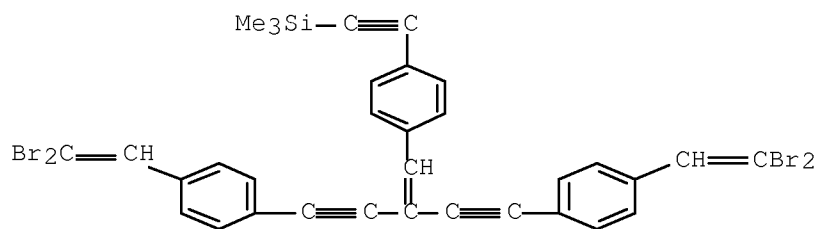


PAGE 1-B



CAS Registry Number
206191-72-8 CAPLUS

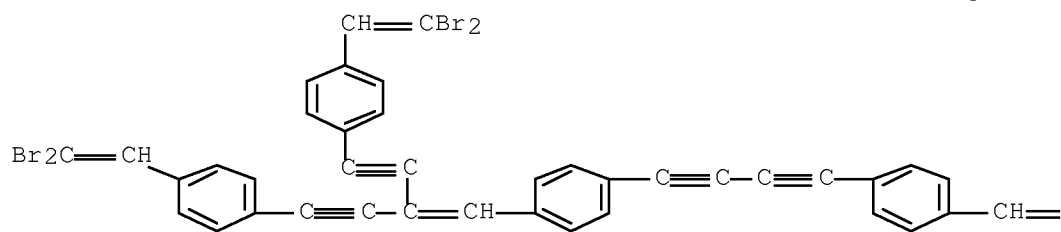
Chemical or Trade Name
Silane, [[4-[4-[4-(2,2-dibromoethenyl)phenyl]~2-[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)



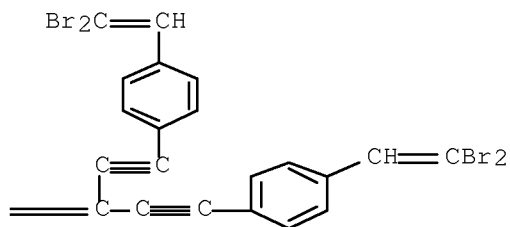
CAS Registry Number
206181-74-0 CAPLUS

Chemical or Trade Name
Benzene, 1,1'-[1,3-butadiyne-1,4-diyl]bis[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



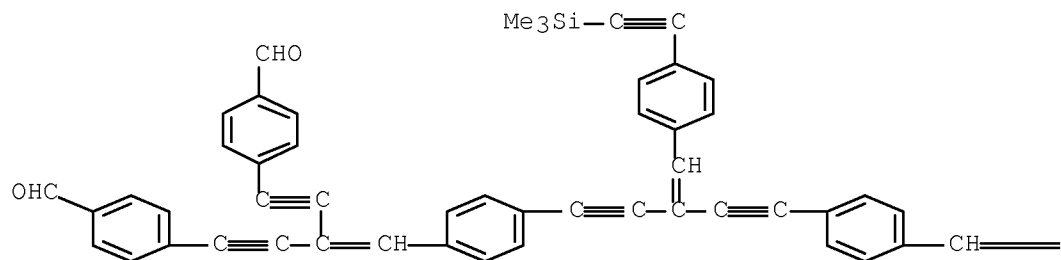
PAGE 1-B

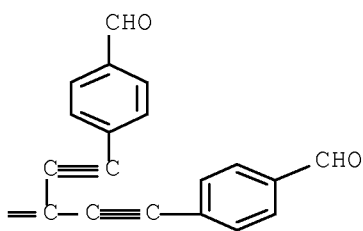


CAS Registry Number
206181-76-2 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[[4-formylphenyl]ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)

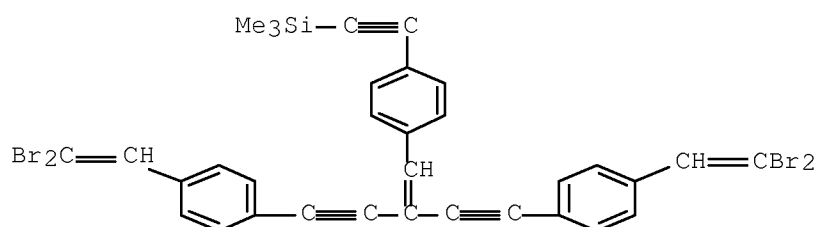
PAGE 1-A





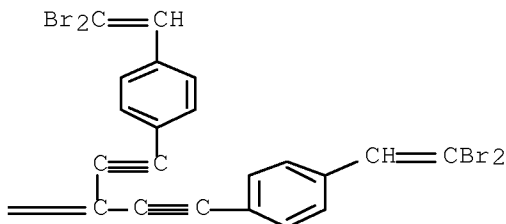
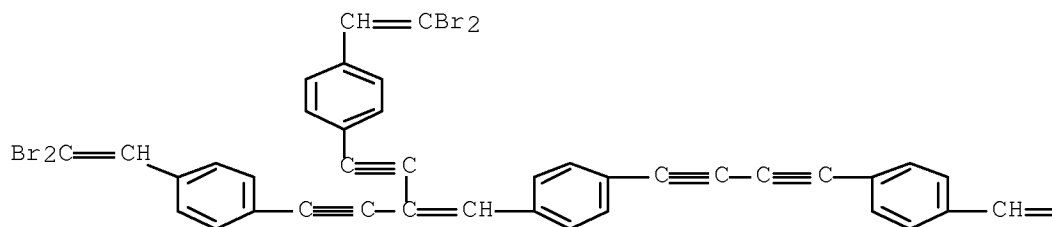
CAS Registry Number
717144-23-5 CAPLUS

Chemical or Trade Name
Silane, [[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-, radical ion(1-) (9CI) (CA INDEX NAME)



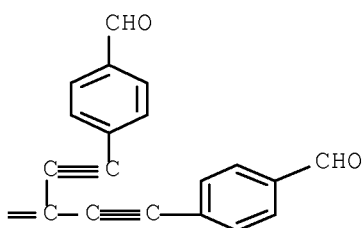
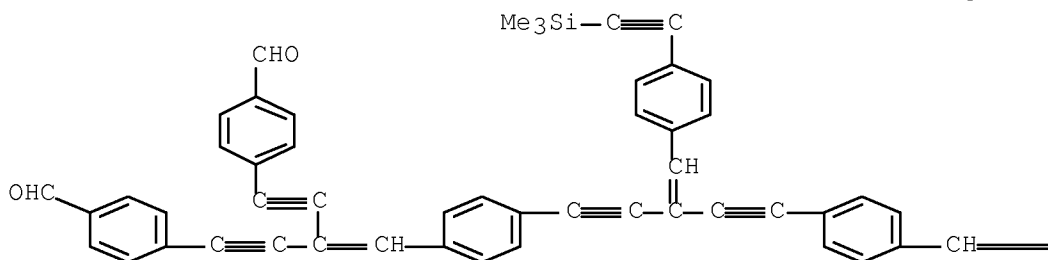
CAS Registry Number
717144-24-6 CAPLUS

Chemical or Trade Name
Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]-, radical ion(1-) (9CI) (CA INDEX NAME)



CAS Registry Number
717144-25-7 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[[3-[[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L3 ANSWER 15 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2004:328526 CAPLUS [Full-text](#)

Document Number

141:54000

Title

Solid-phase synthesis of oligo(triacetylene)s and oligo(phenylenetriacetylene)s employing Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions

Author/Inventor

Utesch, Nils F.; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice

Patent Assignee/Corporate Source

Laboratorium fuer Organische Chemie, ETH-Hoenggerberg, HCI, Zurich, CH-8093, Switz.

Source

Helvetica Chimica Acta (2004), 87(3), 698-718 CODEN: HCACAV; ISSN: 0018-019X

Document Type

Journal

Language

English

Abstract

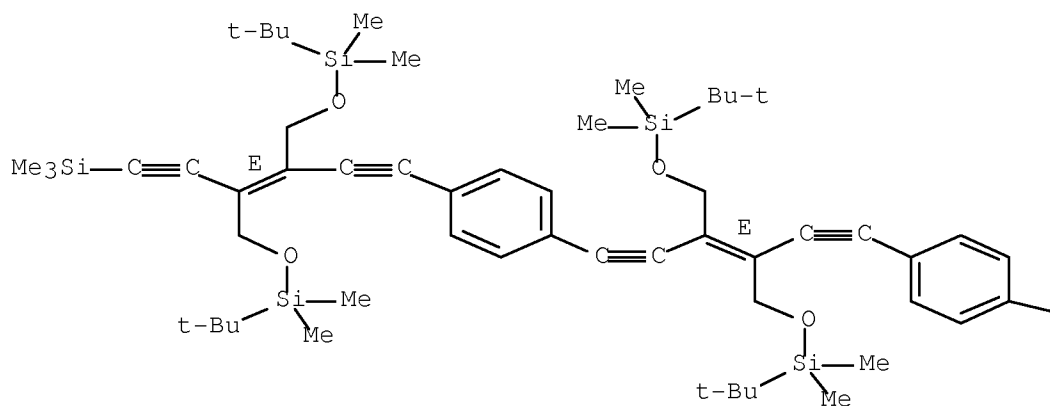
The polymer-supported synthesis of poly(triacetylene)-derived monodisperse oligomers is described, using Pd₀-catalyzed Sonogashira and Cadiot-Chodkiewicz-type cross-couplings as the key steps in the construction of the acetylenic scaffolds. Merrifield resin functionalized with a 1-(4-iodoaryl)triazene linker was chosen as the polymeric support. The linker selection was made based on the results of several model studies in the liquid phase. For the solid-support synthesis of p-[(C₆H₄C.tpbond.CC(CH₂OSiMe₂CM₃);C(CH₂OSiMe₂CM₃);C.tpbond.C)nSiMe₃] [I, n = 2-4] a set of only three reactions was required: (i) Pd₀-catalyzed Sonogashira cross-coupling, (ii) Me₃Si-alkyne deprotection by protodesilylation, and (iii) cleavage of the linker with liberation of I. The longest-wavelength absorption maxima of I [n = 1-4] shift bathochromically with increasing oligomeric length, from λ_{max} 337 nm (I, n = 1) to 384 nm (I, n = 4). Based on the electronic absorption data, the effective conjugation length (ECL) of the oligo(phenylene triacetylene)s is estimated to involve at least four monomer units and 40 C-atoms. π-Electron conjugation in these oligomers is less efficient than in Me₃Si[(C₆H₄C.tpbond.CC(CH₂OSiMe₂CM₃);C(CH₂OSiMe₂CM₃);C.tpbond.C)nSiMe₃] (II) due to poor transmittance of π-electron delocalization by the Ph rings inserted into the oligomeric backbone. Similar conclusions were drawn from the electrochem. properties of the two oligomeric series as determined by cyclic (CV) and rotating-disk voltammetry. In sharp contrast to II, I are strongly fluorescent, with the highest quantum yield Φ_F = 0.69 measured for I [n = 3]. Whereas the Sonogashira cross-coupling on solid support proceeded smoothly, optimal conditions for alkyne-alkyne cross-coupling reactions employing Pd₀-catalyzed Cadiot-Chodkiewicz conditions still remain to be developed.

Hit Structure

CAS Registry Number
554459-62-0 CAPLUS

Chemical or Trade Name

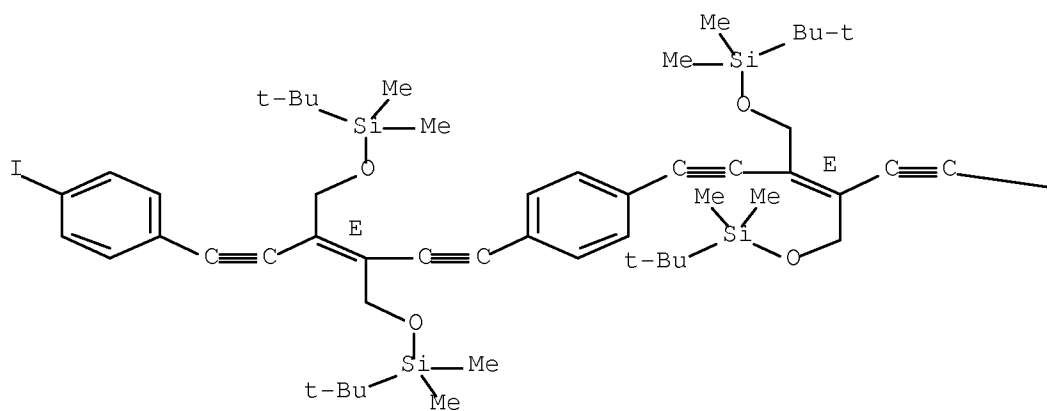
4,9-Dioxo-3,10-disiladodec-6-ene, 6-[[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

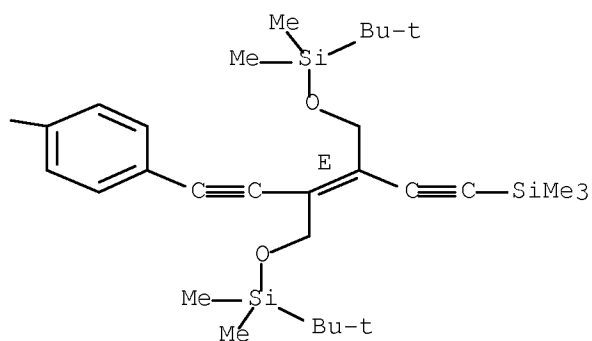


— I

CAS Registry Number
554459-63-1 CAPLUS

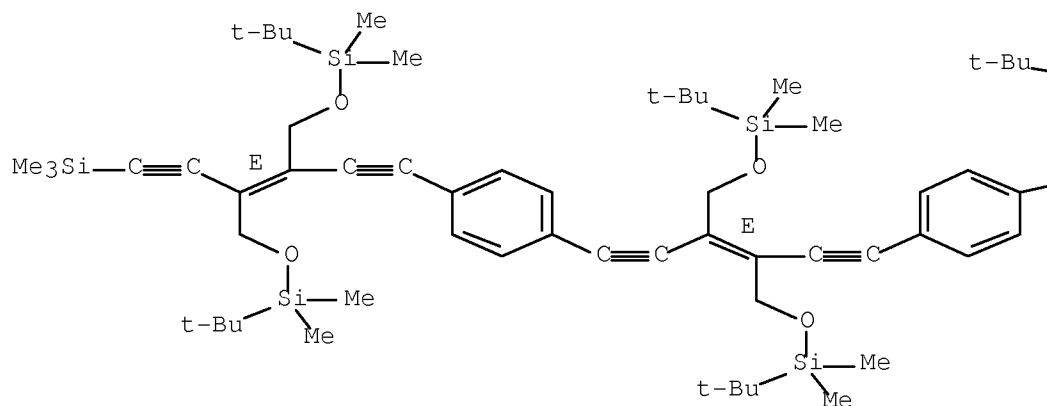
Chemical or Trade Name
4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[[trimethylsilyl]ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

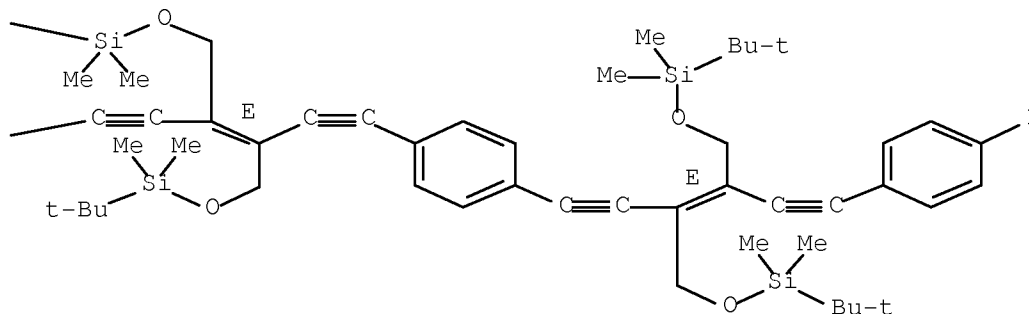




CAS Registry Number
554459-64-2 CAPLUS

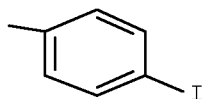
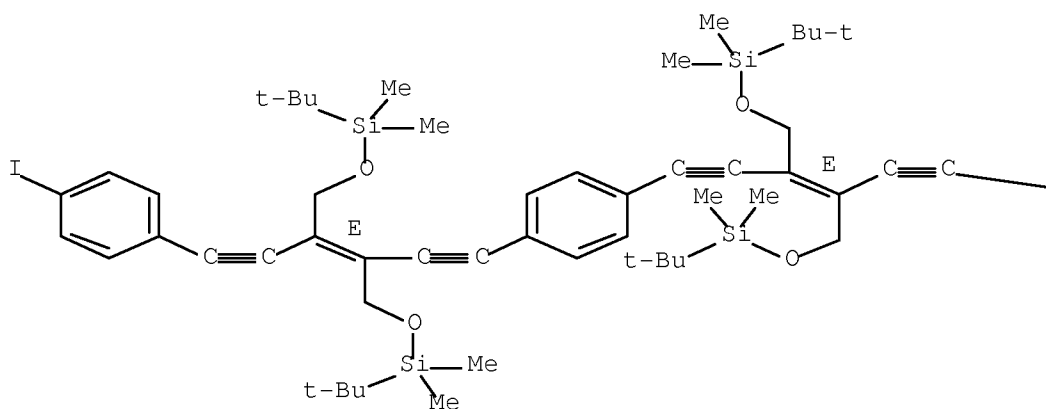
Chemical or Trade Name
4,9-Dioxo-3,10-disiladodeco-6-ene, 6-[[4-[(3E)-6-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)





CAS Registry Number
704916-29-0 CAPLUS

Chemical or Trade Name
4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylenedi-2,1-ethynediyl)bis[7-[(4-iodophenyl)ethynyl]-2,2,3,10,10,11,11-octamethyl-, (6E,6'E)-(9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD
(8 CITINGS)

, L3 ANSWER 16 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2003:491916 CAPLUS [Full-text](#)

Document Number

139:395637

Title

Synthesis of differentially protected/functionalised acetylenic building blocks from p-benzoquinone and their use in the synthesis of new enedynes

Author/Inventor

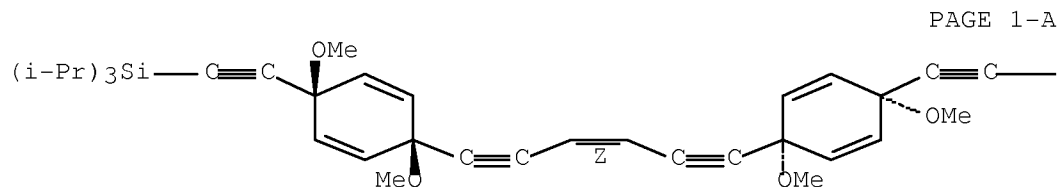
Sankararaman, Sethuraman; Srinivasan, Manivannan
 Patent Assignee/Corporate Source
 Department of Chemistry, Indian Institute of Technology Madras, Madras, 600 036, India
 Source
 Organic & Biomolecular Chemistry (2003), 1(13), 2388-2392 CODEN: OBCRAK; ISSN: 1477-0520
 Document Type
 Journal
 Language
 English

Abstract Sequential addition of two different lithium acetylides to p-benzoquinone yielded diastereomeric mixts. of 1,4-diethynylcyclohexa-2,5-diene-1,4-diols I [R = (Me2CH)3Si, (EtO)2CH] with different protective/functional groups on the two ethynyl groups. Selective monodeprotection of the di-Me ethers of I to the corresponding terminal acetylenes followed by Pd(0)-mediated coupling with (Z)-1,2-dichloroethene yielded new enediyne II bearing cyclohexa-2,5-diene units.

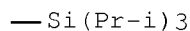
Hit Structure

CAS Registry Number
 626235-20-9 CAPLUS

Chemical or Trade Name
 Silane, [(3Z)-3-hexene-1,5-diyne-1,6-diylbis[(cis-1,4-dimethoxy-2,5-cyclohexadiene-1,4-diyl)-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

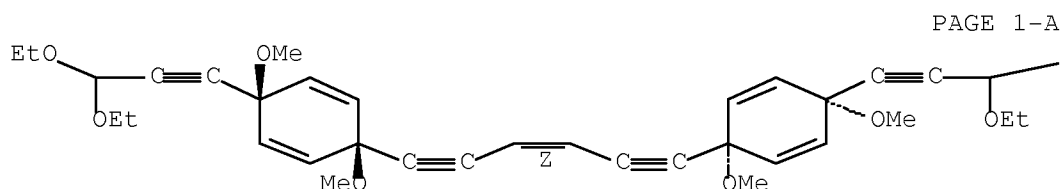


PAGE 1-B



CAS Registry Number
 626235-21-0 CAPLUS

Chemical or Trade Name
 1,4-Cyclohexadiene, 3,3'-(3Z)-3-hexene-1,5-diyne-1,6-diylbis[6-(3,3-diethoxy-1-propynyl)-3,6-dimethoxy-, (cis,cis)- (9CI) (CA INDEX NAME)

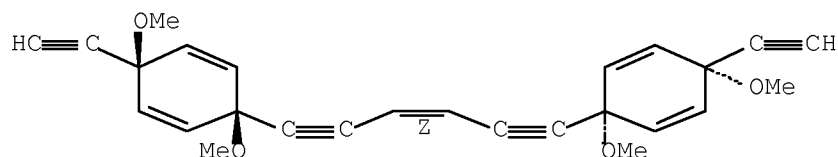


PAGE 1-B



CAS Registry Number
 626235-22-1 CAPLUS

Chemical or Trade Name
 1,4-Cyclohexadiene, 3,3'-(3Z)-3-hexene-1,5-diyne-1,6-diylbis[6-ethynyl-3,6-dimethoxy-, (cis,cis)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
 (6 CITINGS)

Accession Number

2003:234291 CAPLUS [Full-text](#)

Document Number

139:85055

Title

Acetylenic scaffolding on solid support: Poly(triacetylene)-derived oligomers by Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions

Author/Inventor

Utesch, Nils F.; Diederich, Francois

Patent Assignee/Corporate Source

Laboratorium für Organische Chemie, ETH-Honggerberg, HCI, Zurich, CH-8093, Switz.

Source

Organic & Biomolecular Chemistry (2003), 1(2), 237-239 CODEN: OBCRAK; ISSN: 1477-0520

Document Type

Journal

Language

English

Abstract

Synthesis of poly(triacetylene)-derived oligomers by Pd(0)-catalyzed Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions on solid support is reported. Oligo(phenylene triacetylene)s, e.g., $\{[4\text{-C}_6\text{H}_4\text{C}(\text{t-Bu})\text{Si}(\text{Me})_2\text{O}]\}_n$ (R = CH₂OSiMe₂ButMe₂, n = 1, 2, 3, 4) members of a new class of linearly π -conjugated oligomers with all-C backbones, feature very high fluorescence intensities.

Hit Structure

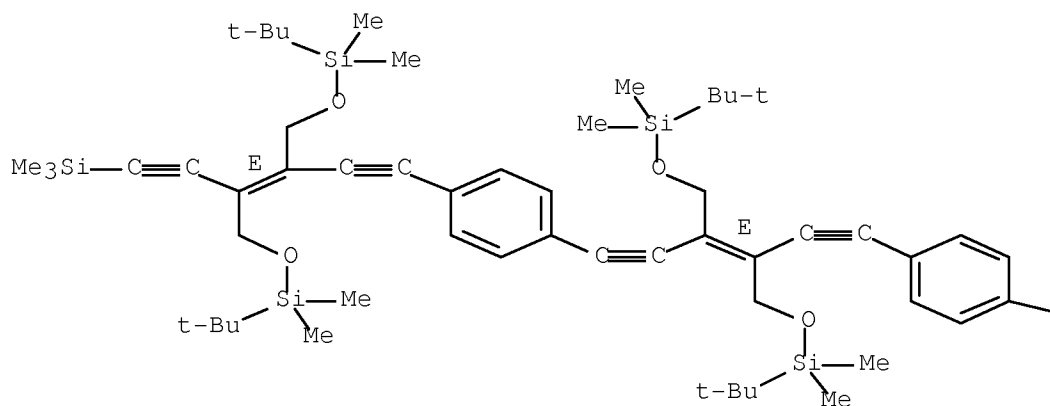
CAS Registry Number

554459-62-0 CAPLUS

Chemical or Trade Name

4,9-Dioxo-3,10-disiladodec-6-ene, 6-[[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[[[trimethylsilyl]ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

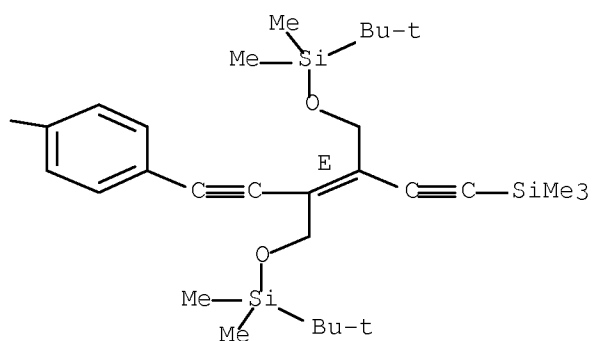
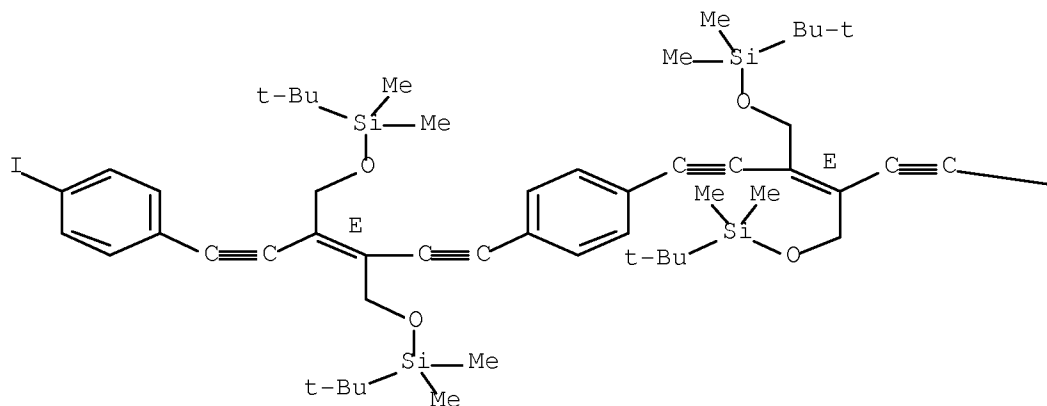
— I

CAS Registry Number

554459-63-1 CAPLUS

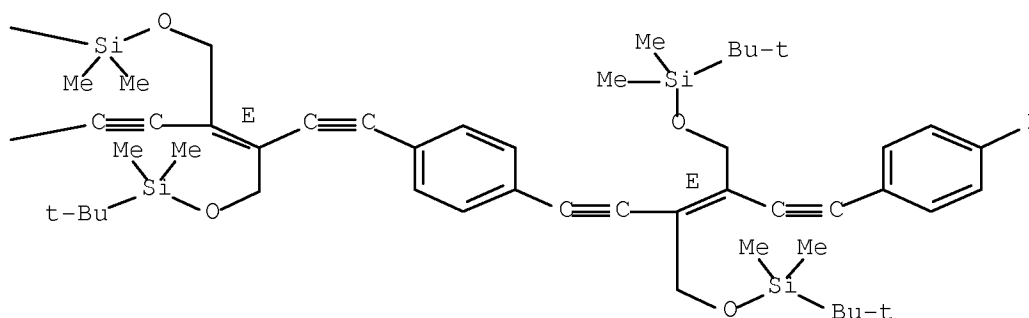
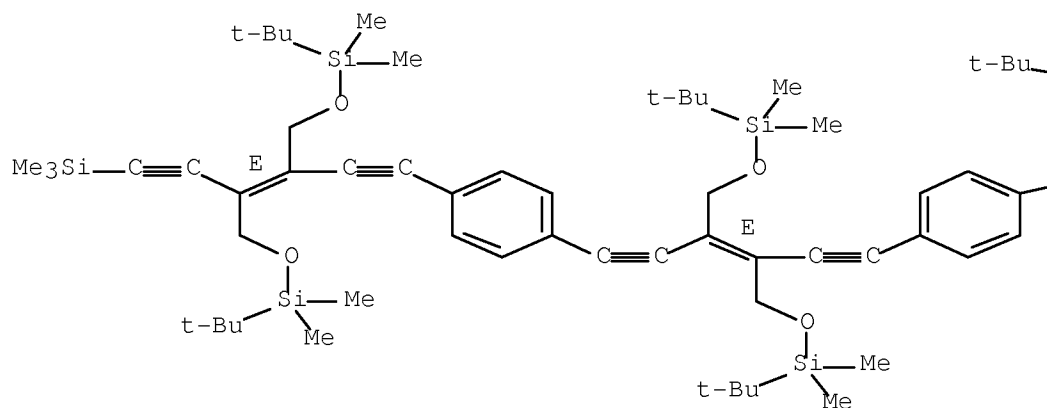
Chemical or Trade Name

4,9-Dioxo-3,10-disiladodec-6-ene, 6-[[[4-[(3E)-6-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[[[trimethylsilyl]ethynyl]-, (6E)- (9CI) (CA INDEX NAME)



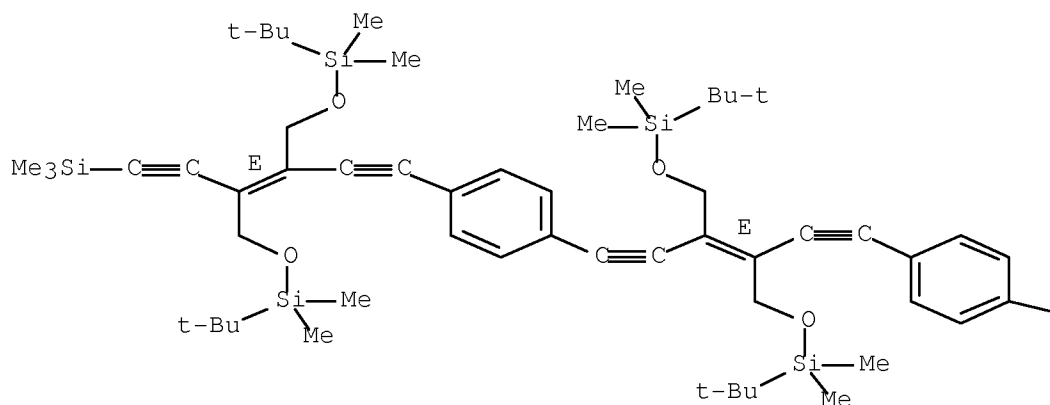
CAS Registry Number
554459-64-2 CAPLUS

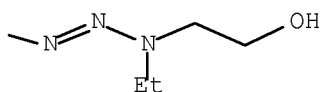
Chemical or Trade Name
4,9-Dioxo-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)



CAS Registry Number
554459-71-1 CAPLUS

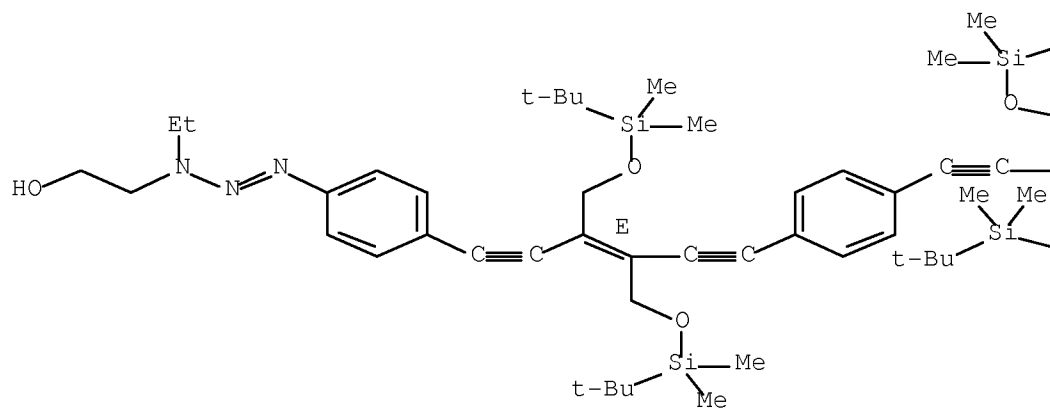
Chemical or Trade Name
Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazen-1-yl]- (CA INDEX NAME)

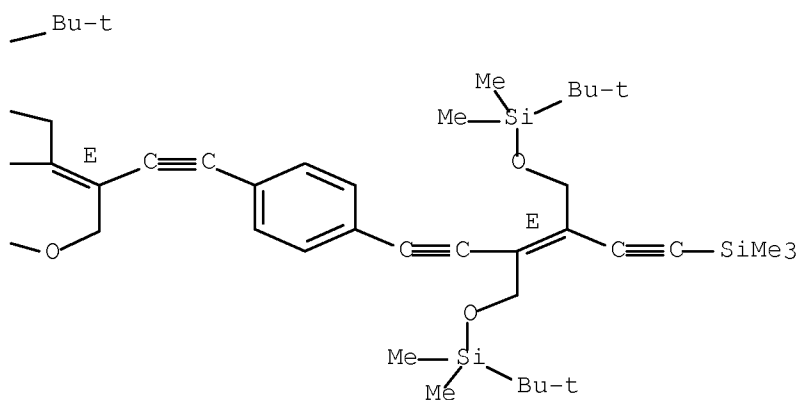




CAS Registry Number
554459-72-2 CAPLUS

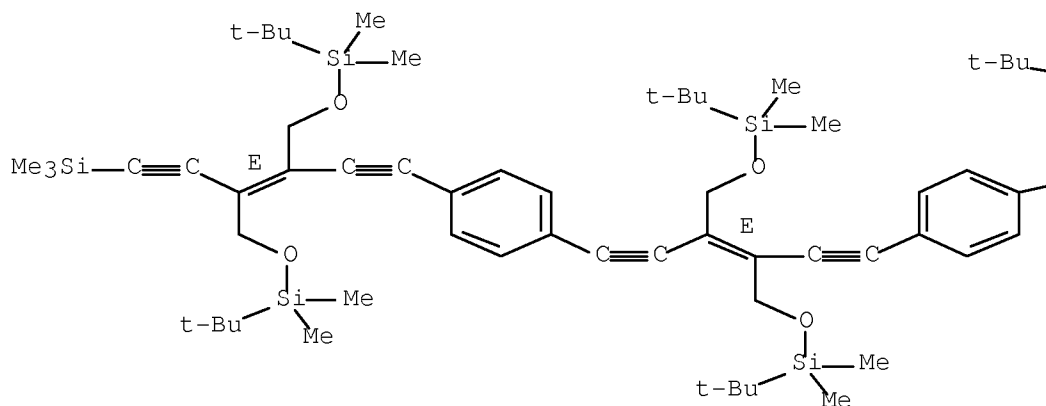
Chemical or Trade Name
Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazen-1-yl]- (CA INDEX NAME)





CAS Registry Number
554459-73-3 CAPLUS

Chemical or Trade Name
Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-6-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazen-1-yl]- (CA INDEX NAME)



L3 ANSWER 18 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Document Number
137:208374

Source
U.S. Pat. Appl. Publ. 26 pp. CODEN: USXXCO

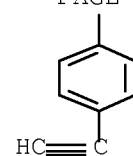
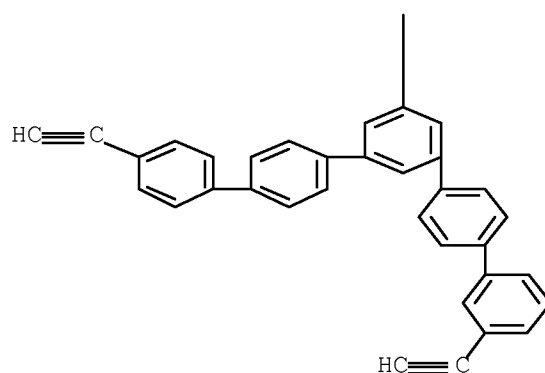
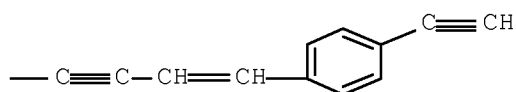
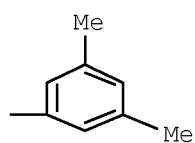
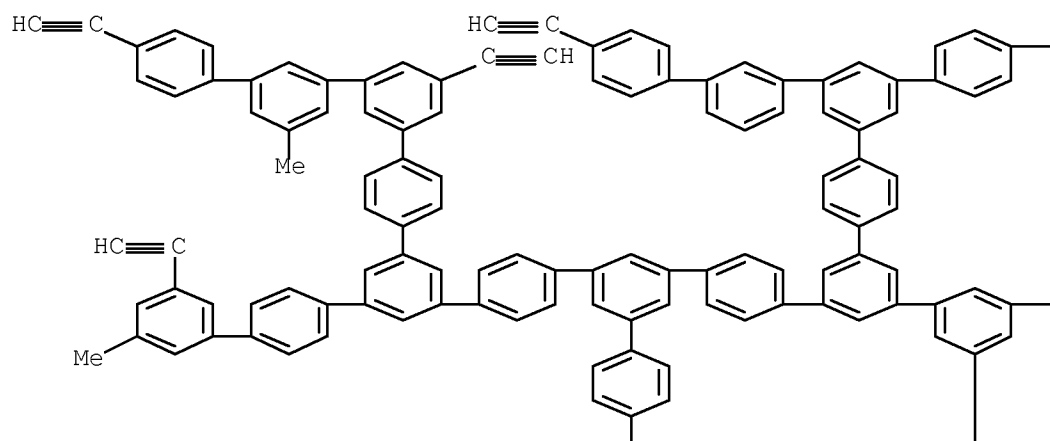
Language
English

English
Patent Information

Abstract

Hit Structure

[illegible]



2002:198497 CAPLUS Full-text

Document Number
136:401857

Title
Acetylide-Bridged Organometallic Oligomers via the Photochemical Metathesis of Methyl-Iron(II) Complexes

Author/Inventor
Field, Leslie D.; Turnbull, Anthony J.; Turner, Peter

Patent Assignee/Corporate Source
School of Chemistry, The University of Sydney, Sydney, 2006, Australia

Source
Journal of the American Chemical Society (2002), 124(14), 3692-3702 CODEN: JACSAT; ISSN: 0002-7863

Document Type
Journal

Language
English

Abstract

The acetylide Me iron(II) complexes, $\text{cis-}[\text{Fe}(\text{dmpe})_2(\text{C.tpbond.CR})(\text{CH}_3)]$ (1) and $\text{trans-}[\text{Fe}(\text{depe})_2(\text{C.tpbond.CR})(\text{CH}_3)]$ (2) (dmpe = 1,2-dimethylphosphinoethane; depe = 1,2-diethylphosphinoethane), were synthesized by transmetalation from the corresponding alkyl halide complexes. Acetylide Me iron(II) complexes were also formed by transmetalation from the chloride complexes, $\text{trans-}[\text{Fe}(\text{dmpe})_2(\text{C.tpbond.CR})(\text{Cl})]$ or $\text{trans-}[\text{Fe}(\text{depe})_2(\text{C.tpbond.CR})(\text{Cl})]$. The structure of $\text{trans-}[\text{Fe}(\text{dmpe})_2(\text{C.tpbond.CC}_6\text{H}_5)(\text{CH}_3)]$ (1a) was determined by single-crystal x-ray diffraction. The Me acetylide iron complexes, $[\text{Fe}(\text{dmpe})_2(\text{C.tpbond.CR})(\text{CH}_3)]$ (1), are thermally stable in the presence of acetylenes; however, under UV irradiation, methane is lost with the formation of a metal bisacetylide. Photochem. metathesis of cis- or $\text{trans-}[\text{Fe}(\text{dmpe})_2(\text{CH}_3)(\text{C.tpbond.CR})]$ ($\text{R} = \text{C}_6\text{H}_5$ (1a), 4-C₆H₄OCH₃ (1b) with terminal acetylenes was used to selectively synthesize unsym. substituted iron(II) bisacetylide complexes of the type $\text{trans-}[\text{Fe}(\text{dmpe})_2(\text{C.tpbond.CR})(\text{C.tpbond.CR}')] [\text{R} = \text{Ph}$, $\text{R}' = \text{Ph}$ (6a), 4-CH₃OC₆H₄ (6b), tBu (6c), SiMe₃ (6d), (CH₂)₄C.tpbond.CH (6e); $\text{R} = 4\text{-CH}_3\text{OC}_6\text{H}_4$, $\text{R}' = 4\text{-CH}_3\text{OC}_6\text{H}_4$, (6g), tBu (6h), (CH₂)₄C.tpbond.CH (6i), adamantyl (6j)]. The structure of the unsym. iron(II) bisacetylide complex $\text{trans-}[\text{Fe}(\text{dmpe})_2(\text{C.tpbond.CC}_6\text{H}_5)(\text{C.tpbond.CC}_6\text{H}_4\text{OCH}_3)]$ (6b) was determined by single-crystal x-ray diffraction. The photochem. metathesis of the bis-acetylene, 1,7-octadiyne, with $\text{trans-}[\text{Fe}(\text{dmpe})_2(\text{CH}_3)(\text{C.tpbond.CPh})]$ (1a), was utilized to synthesize the bridged binuclear species $\text{trans,trans-}[(\text{C}_6\text{H}_5\text{C.tpbond.C})\text{Fe}(\text{dmpe})_2(\mu\text{-C.tpbond.C}(\text{CH}_2)_4\text{C.tpbond.C})\text{Fe}(\text{dmpe})_2(\text{C.tpbond.CC}_6\text{H}_5)]$ (11). The trinuclear species $\text{trans,trans,trans-}[(\text{C}_6\text{H}_5\text{C.tpbond.C})\text{Fe}(\text{dmpe})_2(\mu\text{-C.tpbond.C}(\text{CH}_2)_4\text{C.tpbond.C})\text{Fe}(\text{dmpe})_2(\mu\text{-C.tpbond.C}(\text{CH}_2)_4\text{C.tpbond.C})\text{Fe}(\text{dmpe})_2(\mu\text{-C.tpbond.C}(\text{CH}_2)_4\text{C.tpbond.C})\text{Fe}(\text{dmpe})_2(\text{C.tpbond.CC}_6\text{H}_5)]$ (12) was synthesized by the photochem. reaction of $\text{Fe}(\text{dmpe})_2(\text{C.tpbond.CPh})(\text{C.tpbond.C}(\text{CH}_2)_4\text{C.tpbond.CH})$ (6a) with $\text{Fe}(\text{dmpe})_2(\text{CH}_3)_2$. Extended irradiation of the bisacetylide complexes with phenylacetylene resulted in insertion of the terminal alkyne into one of the metal acetylide bonds to give acetylide butenyne complexes. The structure of the acetylide butenyne complex, $\text{trans-}[\text{Fe}(\text{dmpe})_2(\text{C.tpbond.CC}_6\text{H}_4\text{OCH}_3)(\eta^1\text{-C}(\text{C}_6\text{H}_5)\text{CH}(\text{C.tpbond.CC}_6\text{H}_4\text{OCH}_3))]$ (9a) was determined by single-crystal x-ray diffraction.

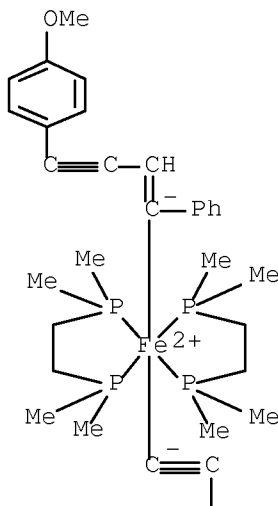
Hit Structure

CAS Registry Number
425390-70-7 CAPLUS

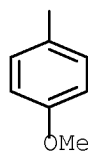
Chemical or Trade Name

Iron, bis[1,2-ethanediyldibis(dimethylphosphine-κP)][(4-methoxyphenyl)ethynyl][(1E)-4-(4-methoxyphenyl)-1-phenyl-1-buten-3-ynyl]-, (OC-6-11)- (9CI) (CA INDEX NAME)

PAGE 1-A



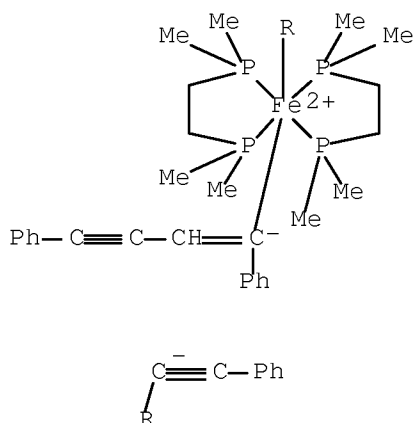
PAGE 2-A



CAS Registry Number
425390-85-4 CAPLUS

Chemical or Trade Name

Iron, [(1E)-1,4-diphenyl-1-buten-3-ynyl]bis[1,2-ethanediyldibis(dimethylphosphine-κP)](phenylethynyl)-, (OC-6-11)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)

L3 ANSWER 20 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2001:714296 CAPLUS [Full-text](#)

Document Number

136.69640

Title

Synthesis and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units

Author/Inventor

Wan, W. Brad; Chiechi, Ryan C.; Weakley, Timothy J. R.; Haley, Michael M.

Patent Assignee/Corporate Source

Department of Chemistry and the Materials Science Institute, University of Oregon, Eugene, OR, 97403-1253, USA

Source

European Journal of Organic Chemistry (2001), (18), 3485-3490 CODEN: EJOCFK; ISSN: 1434-193X

Document Type

Journal

Language

English

Abstract

Dehydrobenzoannulene derivs. containing isolated alkene linkages, e.g., I, were synthesized by combining an in situ Pd/Cu-mediated cross-coupling with an intramol. cyclization strategy. ¹H NMR studies of these macrocycles and comparison with related systems verify that highly alkynylated dehydrobenzoannulenes possess weak induced ring currents, indicative of aromatic (4n+2 π systems) and antiarom. (4n π systems) behavior, in spite of their large size and extensive benzannulation.

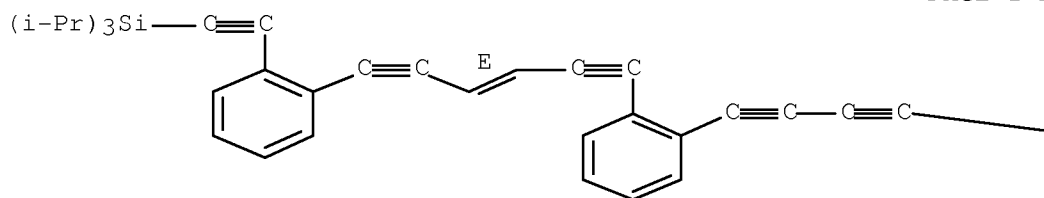
Hit Structure

CAS Registry Number

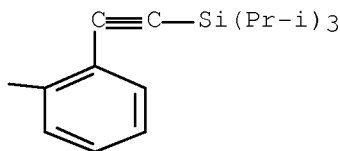
214628-17-8 CAPLUS

Chemical or Trade Name

Silane, tris(1-methylethyl)[[2-[(3E)-6-[2-[4-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-1,3-butadiynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)



PAGE 1-A



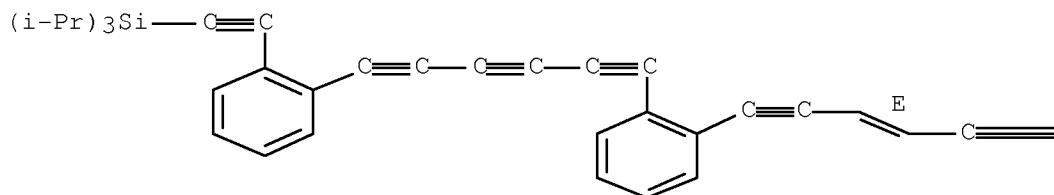
PAGE 1-B

CAS Registry Number

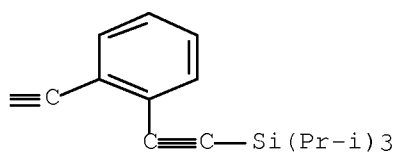
214628-18-9 CAPLUS

Chemical or Trade Name
 Silane, tris(1-methylethyl)[[2-[6-[2-[(3E)-6-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]-1,3,5-hexatriynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



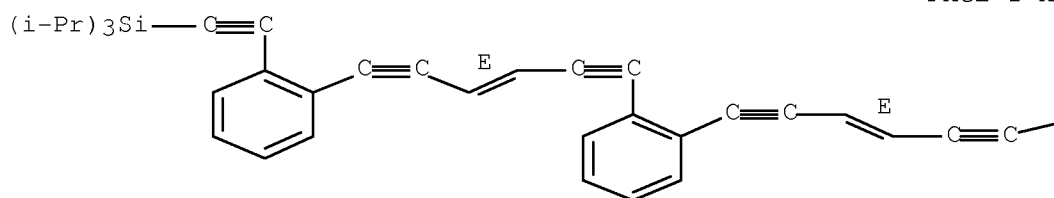
PAGE 1-B



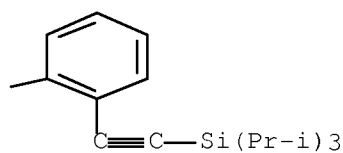
CAS Registry Number
 383404-38-4 CAPLUS

Chemical or Trade Name
 Silane, [1,2-phenylenebis[(3E)-3-hexene-1,5-diyne-6,1-diyl-2,1-phenylene-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L3 ANSWER 21 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2000:832492 CAPLUS [Full-text](#)

Document Number

134:310920

Title

Bis(enediyne) Macrocycles: Synthesis, Reactivity, and Structural Analysis

Author/Inventor

Blanchette, H. S.; Brand, S. C.; Naruse, H.; Weakley, T. J. R.; Haley, M. M.

Patent Assignee/Corporate Source

Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA

Source

Tetrahedron (2000), 56(49), 9581-9588 CODEN: TETRAB; ISSN: 0040-4020

Document Type

Journal

Language

English

Abstract

The authors describe the syntheses of five macrocycles possessing two enediyne warheads, along with the structural and thermal analyses of these bis(enediyne) compds. The solid-state packing of one of the compds. suggests the possibility for the mol. to undergo a topochem. diacetylene polymerization

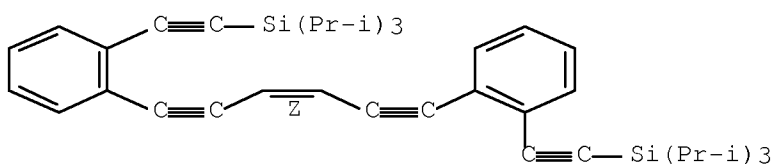
Hit Structure

CAS Registry Number

335378-20-6 CAPLUS

Chemical or Trade Name

Silane, [(3Z)-3-hexene-1,5-diyne-1,6-diylbis(2,1-phenylene-2,1-ethynediyl)]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)]

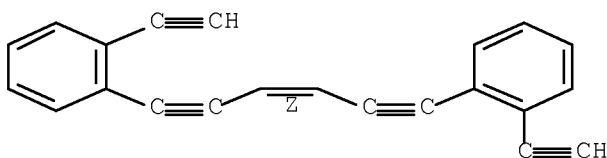


CAS Registry Number

335378-30-8 CAPLUS

Chemical or Trade Name

Benzene, 1,1'-(3Z)-3-hexene-1,5-diyne-1,6-diylbis[2-ethynyl- (9CI) (CA INDEX NAME)]



OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)

L3 ANSWER 22 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2000:767122 CAPLUS [Full-text](#)

Document Number

134:71381

Title

Synthesis and structure of a new [6.6]metacyclophane with enediyne bridges

Author/Inventor

Srinivasan, Manivannan; Sankararaman, Sethuraman; Dix, Ina; Jones, Peter G.

Patent Assignee/Corporate Source

Department of Chemistry, Indian Institute of Technology, Madras, 600 036, India

Source

Organic Letters (2000), 2(24), 3849-3851 CODEN: ORLEF7; ISSN: 1523-7060

Document Type

Journal

Language

English

Abstract

Synthesis and structure of a novel [6.6]metacyclophane with enediyne bridges I is reported. I was prepared by reacting 1,3-diethynylbenzene with EtMgBr/THF and DMF to give the monoaldehyde. The monoaldehyde was subsequently converted to the acetal, coupled with ClCH₂CHCl to give bis-acetal, which was hydrolyzed to the dialdehyde II. II underwent McMurry coupling using TiCl₃ and Zn-Cu couple in DME to give I in 69% yield.

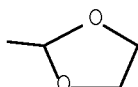
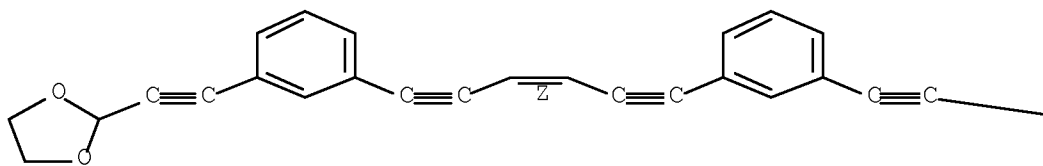
Hit Structure

CAS Registry Number

315716-90-6 CAPLUS

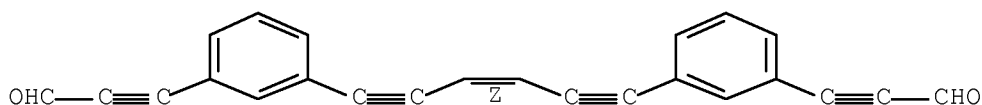
Chemical or Trade Name

1,3-Dioxolane, 2,2'-[(3Z)-3-hexene-1,5-diyne-1,6-diylbis(3,1-phenylene-2,1-ethynediyl)]bis- (9CI) (CA INDEX NAME)



CAS Registry Number
315716-91-7 CAPLUS

Chemical or Trade Name
2-Propynal, 3,3'-[3,3'-bis(2-propynyl)-1,5-diyne-1,5-diyne-1,6-diyldi-3,1-phenylene]bis-
(9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS
RECORD (18 CITINGS)

L3 ANSWER 23 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1999:673316 CAPLUS Full-text

Document Number

131:337589

Title

Electronic structure of fully conjugated dendritic oligomers of β,β -dibromo-4-ethynyl styrene

Author/Inventor

Fomine, Serguei; Fomina, Lioudmila; Guadarrama, Patricia

Patent Assignee/Corporate Source

Universidad Nacional Autonoma Mexico, Inst de Investigaciones en Materiales, Coyoacan, 04510 CU, Mex.

Source

Journal of Molecular Structure: THEOCHEM (1999), 488, 207-216 CODEN: THEODJ; ISSN: 0166-1280

Document Type

Journal

Language

English

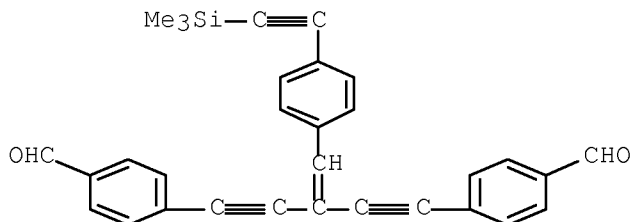
Abstract

Quantum-mech. calcns. of fully conjugated dendritic oligomers carried out at B3LYP/3-21G//HF/3-21G (d) and B3LYP/3-21G//PM3 levels of theory showed that loose dendritic architecture of β,β -dibromo-4-ethynyl styrene oligomers contributes little to the instability and conjugation disruption compared to 1 \rightarrow 2 branched polyacetylene, while Br terminal atoms in dendrimers strongly affect the electronic d. distribution in studied mols. On the one hand the bulky bromine atoms decrease the conjugation in Br-terminated dendrimers caused by steric hindrances, on the other hand, highly polarizable bromine atoms reduced significantly adiabatic ionization potentials (IPa) to be up to 1.5 eV lower than corresponding vertical potentials (IPv). Another phenomenon contributing to the reducing of IPa's of all dendrimers is the flattening of mol. geometry accompanying the ionization thus allowing better delocalization of pos. charge over the conjugated system while all aromatic ring except the very outer layer lost their aromaticity becoming essentially quinone by nature.

Hit Structure

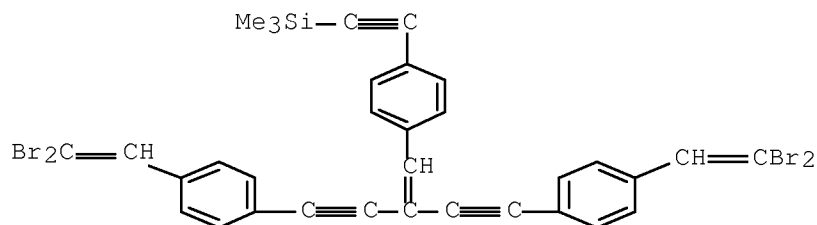
CAS Registry Number
206181-71-7 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[3-[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-
pentadiyne-1,5-diyldi- (9CI) (CA INDEX NAME)



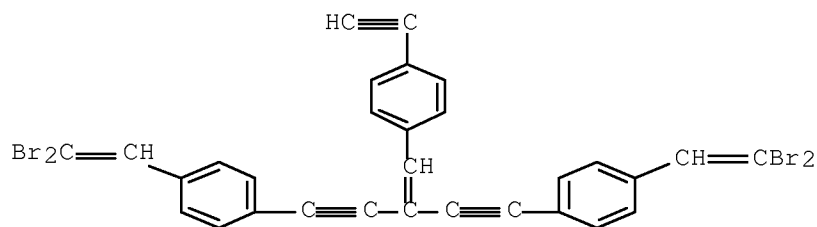
CAS Registry Number
206181-72-8 CAPLUS

Chemical or Trade Name
 Silane, [[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-
 (9CI) (CA INDEX NAME)



CAS Registry Number
 206181-73-9 CAPLUS

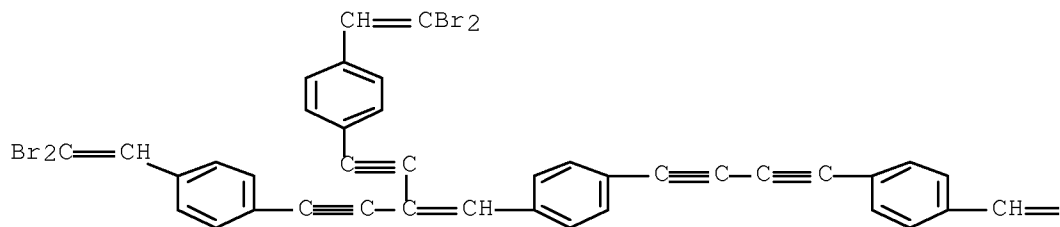
Chemical or Trade Name
 Benzene, 1,1'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[4-(2,2-dibromoethenyl)- (9CI) (CA INDEX NAME)



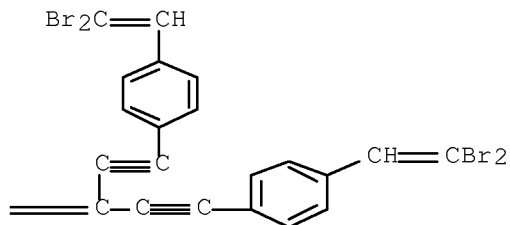
CAS Registry Number
 206181-74-0 CAPLUS

Chemical or Trade Name
 Benzene, 1,1'-[1,3-butadiyne-1,4-diyl]bis[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

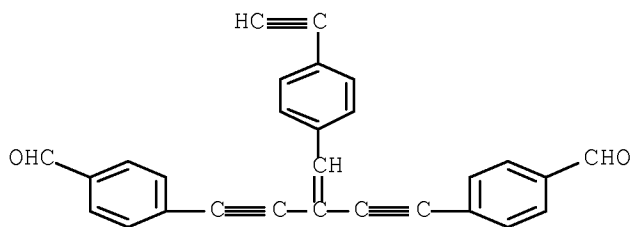


PAGE 1-B



CAS Registry Number
 206181-75-1 CAPLUS

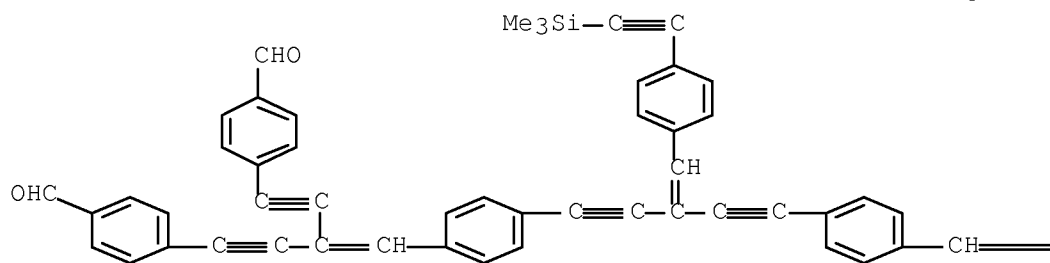
Chemical or Trade Name
 Benzaldehyde, 4,4'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



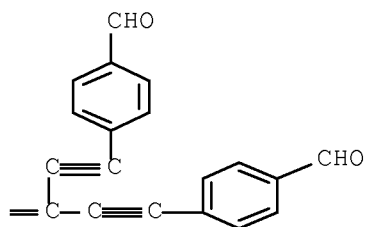
CAS Registry Number
206181-76-2 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)

PAGE 1-A



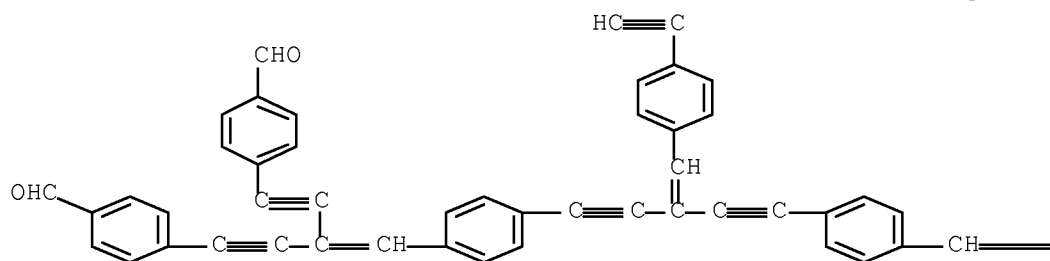
PAGE 1-B

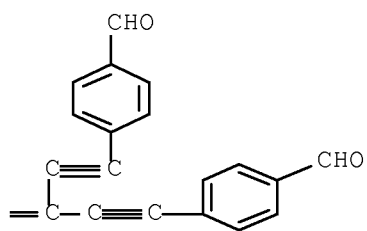


CAS Registry Number
206181-77-3 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[[3-[[4-ethynylphenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)

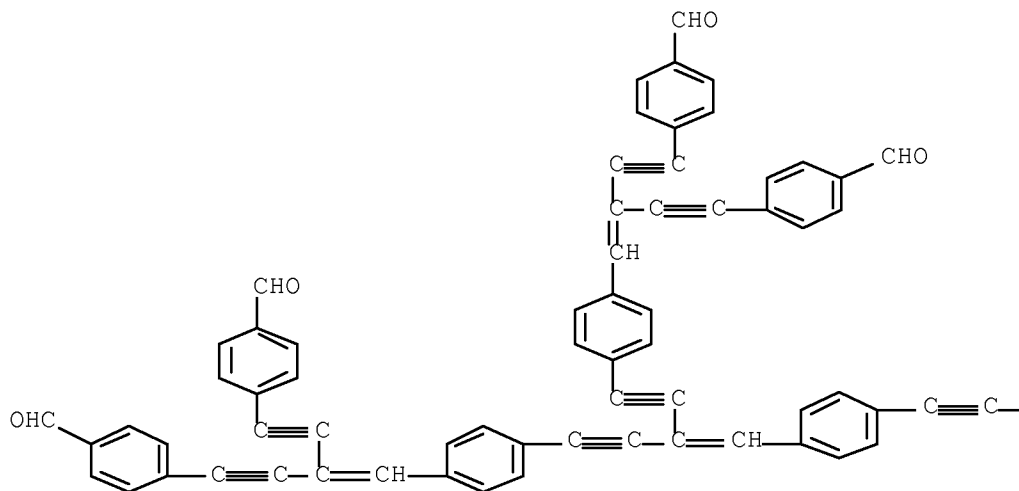
PAGE 1-A

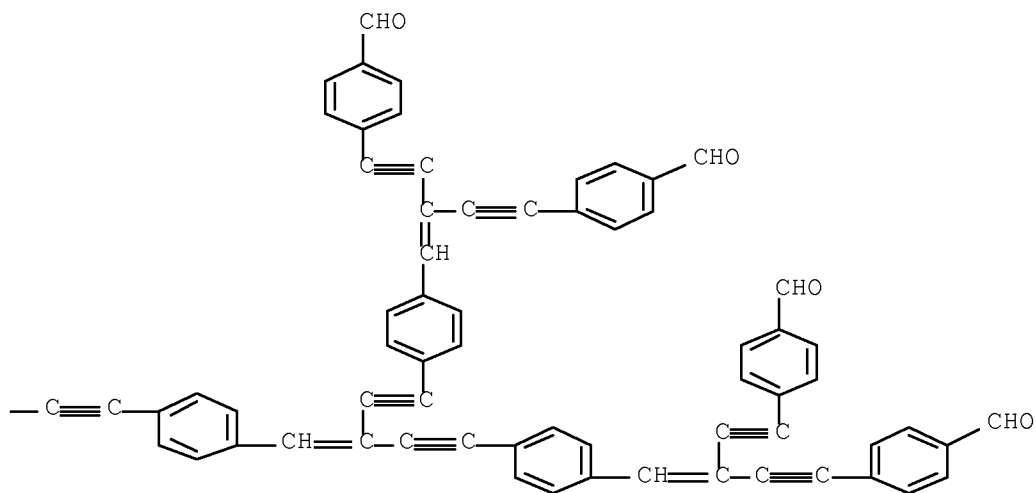




CAS Registry Number
206181-78-4 CAPLUS

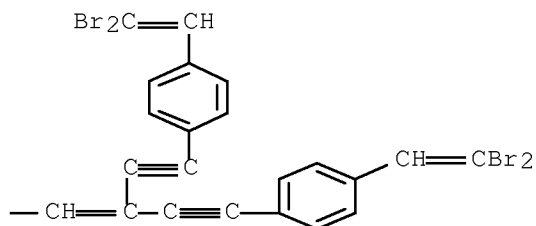
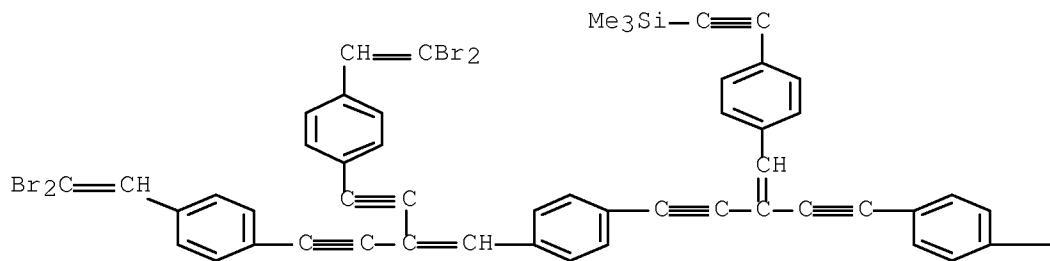
Chemical or Trade Name
Benzaldehyde, 4,4'-[1,3-butadiyne-1,4-diylbis[4,1-phenylene[3-[[4-(4-formylphenyl)-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-3-buten-1-yne-4,1-diyl]-4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)





CAS Registry Number
206181-79-5 CAPLUS

Chemical or Trade Name
Silane, [[4-[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L3 ANSWER 24 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number
1999-650836 CAPLUS File: 881

Document Number
132:16702

Title

Theoretical description of luminescent effects in β,β -di(4'-formylphenylethynyl)-4-ethynylstyrene

Author/Inventor

Salcedo, R.; Guadarrama, P.; Sansores, L. E.; Fomine, S.; Fomina, L.

Patent Assignee/Corporate Source

Inst. de Investigaciones en Materiales, Inst. de Investigaciones en Materiales, UNAM, Mexico, 04510, Mex.

Source

Materials Research Society Symposium Proceedings (1999), 560(Luminescent Materials), 359-364 CODEN: MRSPDH; ISSN: 0272-9172

Document Type

Journal

Language

English

Abstract

Theor. calcs. at HF/6-31 G(d) level were carried out on fully conjugated compds. (4-ethynylbenzaldehyde, β,β -dibromo-4-ethynylstyrene, β,β -Di(4'-formylphenylethynyl)-4-ethynylstyrene and its dimer) to understand the source of blue emission observed in oligomers of the 1st and 2nd generation in CHCl_3 solns. The frontier orbitals are distributed through the framework of the mols. (benzene rings, double and triple bonds and chromophores). Addnl., a CI approach was applied over β,β -Di(4'-formylphenylethynyl)-4-ethynylstyrene (compound 3) at CIS/6-31 G(d) level to modeling excited states and simulate the UV-visible spectrum exptl. obtained. Calculated transitions corresponded to $S_0 \rightarrow S_1$ which are, presumably, responsible for the fluorescence observed

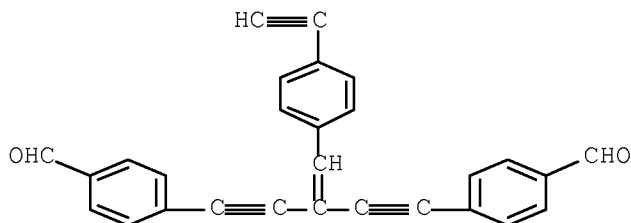
Hit Structure

CAS Registry Number

206181-75-1 CAPLUS

Chemical or Trade Name

Benzaldehyde, 4,4'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)

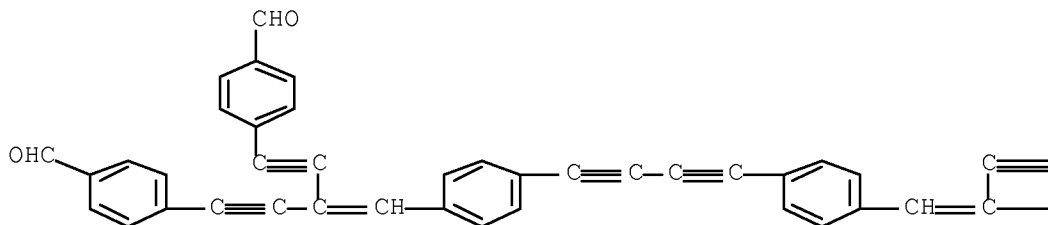


CAS Registry Number

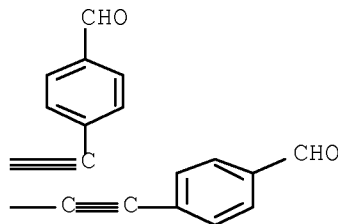
251479-84-2 CAPLUS

Chemical or Trade Name

Benzaldehyde, 4,4'-[1,3-butadiyne-1,4-diylbis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)



PAGE 1-A



PAGE 1-B

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

Accession Number

1998:756297 CAPLUS [Full-text](#)

Document Number

130:118607

Title

Porphyrin-[(E)-1,2-diethynylethene] scaffolding. Synthesis and optical and electrochemical properties of multinanometer-sized porphyrin arrays

Author/Inventor

Wytko, Jennifer; Berl, Volker; McLaughlin, Mark; Tykewinski, Rik R.; Schreiber, Martin; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice

Patent Assignee/Corporate Source

Laboratorium Organische Chemie, ETH-Zentrum, Zurich, CH-8092, Switz.

Source

Helvetica Chimica Acta (1998), 81(11), 1964-1977 CODEN: HCACAV; ISSN: 0018-019X

Document Type

Journal

Language

English

Abstract

Two series of linearly conjugated hybrid materials, consisting of (E)-1,2-diethynylethene (DEE; hex-3-ene-1,5-diyne) and Zn(II) porphyrin components, were prepared by Pd0-catalyzed cross-coupling reactions. In 1 series, 1 or 2 DEE substituents were introduced into the meso-positions of the Zn(II) porphyrins, leading from Zn 5,15-bis[[ethoxycarbonyl]propoxy]phenylporphinate (I) to I and II (n = 1; R = SiMe2tBu). The second series contains the linearly π -conjugated mol. rods III (n = 1-3) that span a length range from 23 Å for III (n = 1) to 53 Å for III (n = 3). The larger rods III (n = 2 and 3) consist of 2 or 3 porphyrin moieties, resp., that are bridged at the meso-positions by trans-enediynediyl (hex-3-ene-1,5-diyne-1,6-diyl) linkers. The UV/VIS spectra in the series I, II, and III (n = 1) showed a strong bathochromic shift of both Soret and Q bands of the Zn(II) porphyrin as a result of the addition of DEE substituents. Upon changing from I to II, the Q band was further bathochromically shifted, whereas the Soret band remained nearly at the same position but became broadened and displayed a shoulder on the lower-wavelength edge as a result of excitonic coupling. The close resemblance between the UV/Vis spectra of III (n = 2 and 3) suggests that saturation of the optical properties in the oligomeric series already occurs at the stage of dimeric III (n = 2). Stationary voltammetric investigations showed that the DEE substituents act as strong electron acceptors which induce large anodic shifts in the 1st reduction potential upon changing from I to II (ΔE = 190 mV) and to III (n = 1) (ΔE = 340 mV). Increasing the number of porphyrin moieties upon changing from III (n = 1) to III (n = 2) had no effect on the 1st reduction potential yet the 1st oxidation potential was substantially lowered (ΔE = 110 mV). Large differences in the potentials for 1-electron oxidation of the 2 porphyrin moieties in III (n = 2) (ΔE = 200 mV) confirmed the existence of substantial electronic communication between the 2 macrocycles across the trans-enediynediyl bridge.

Hit Structure

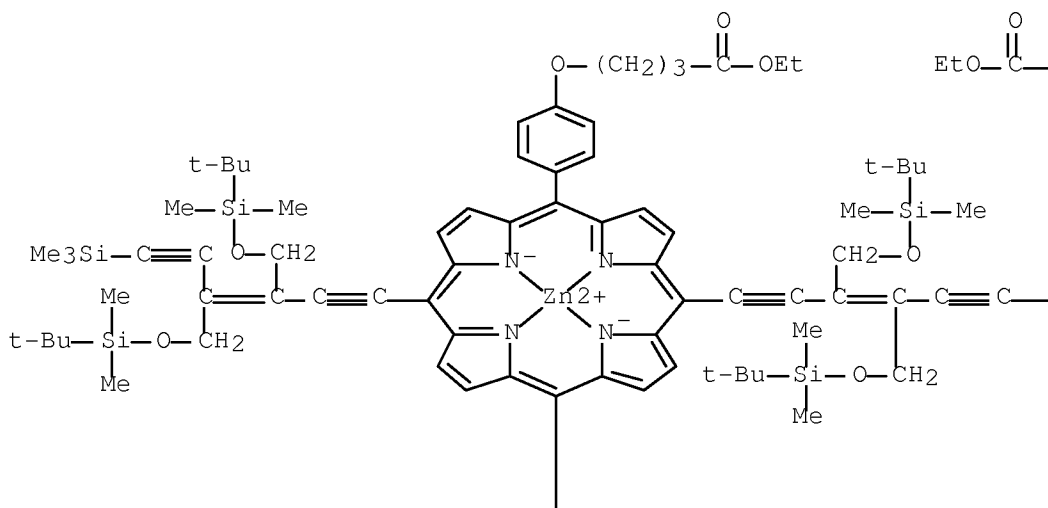
CAS Registry Number

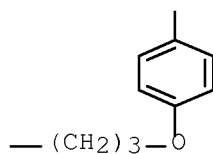
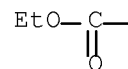
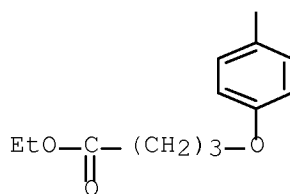
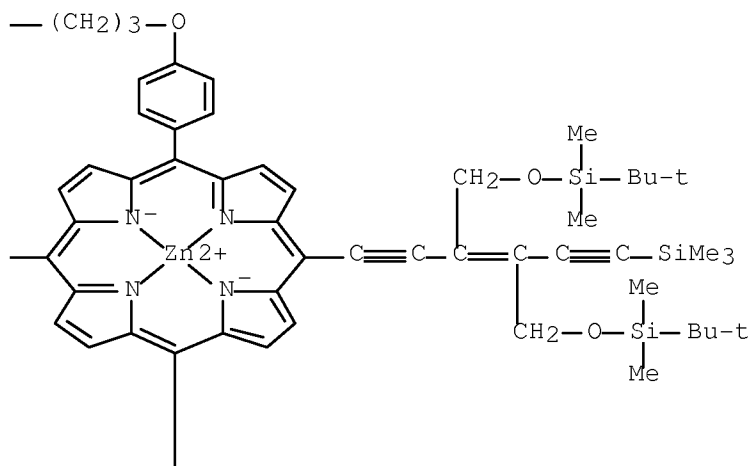
219493-19-9 CAPLUS

Chemical or Trade Name

Zinc, [μ -[[tetraethyl 4,4',4'',4'''-[[[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyne-1,6-diyl]bis[[20-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyne]-21H,23H-porphine-10,5,15-triyl- κ N21, κ N22, κ N23, κ N24]-4,1-phenyleneoxy]]tetrakis[butanoato]](4-)]di- (9CI) (CA INDEX NAME)

PAGE 1-A





OS.CITING REF COUNT: 45 THERE ARE 45 CAPLUS RECORDS THAT CITE THIS RECORD (45 CITINGS)

L3 ANSWER 26 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number
1998:606810 CAPLUS [Full text](#)
Document Number
129:302407

Title
Synthesis of expanded planar dehydrobenzoannulenes: weakly diatropic, weakly paratropic, or atropic?

Author/Inventor
Wan, W. Brad; Kimball, David B.; Haley, Michael M.
Patent Assignee/Corporate Source
Department of Chemistry, University of Oregon, Oregon, 97403-1253, USA

Source
Tetrahedron Letters (1998), 39(38), 6795-6798 CODEN: TELEAY; ISSN: 0040-4039

Document Type
Journal

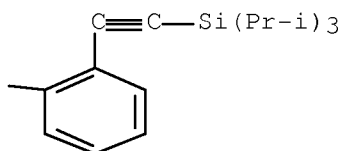
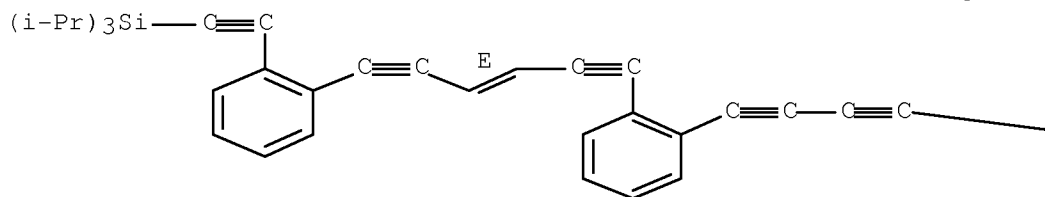
Language
English

Abstract
Use of a Cu/Pd cross-coupling strategy has led to the synthesis of the first dehydrobenzoannulenes I [X = C.tpbond.C, (E)-CH:CH; n = 0,1] containing triacetylenic linkages. NMR studies of these macrocycles and comparison with other known systems indicate that, in spite of their large size and extensive benzannellation, dehydrobenzoannulenes possess weak induced ring currents.

Hit Structure

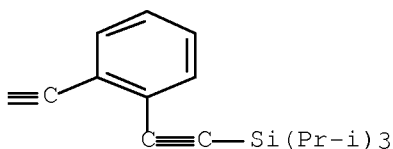
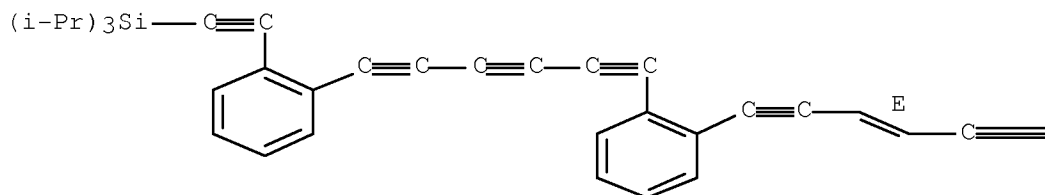
CAS Registry Number
214628-17-8 CAPLUS

Chemical or Trade Name
Silane, tris(1-methylethyl)[[2-[(3E)-6-[2-[4-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-1,3-butadiynyl]phenyl]-3-hexene-1,5-



CAS Registry Number
214628-18-9 CAPLUS

Chemical or Trade Name
Silane, tris(1-methylethyl)[[2-[6-[2-[(3E)-6-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]-1,3,5-hexatriynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 26 THERE ARE 26 CAPLUS RECORDS THAT CITE THIS RECORD (27 CITINGS)

.L3 ANSWER 27 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1998:269262 CAPLUS ~~File 18.1~~

Document Number

128:257221

Title

Steric Hindrance Facilitated Synthesis of Enynes and Their Intramolecular [4 + 2] Cycloaddition with Alkynes

Author/Inventor

Gonzalez, Juan J.; Francesch, Andres; Cardenas, Diego J.; Echavarren, Antonio M.

Patent Assignee/Corporate Source

Departamento de Quimica Organica, Universidad Autonoma de Madrid, Madrid, 28049, Spain

Source

Journal of Organic Chemistry (1998), 63(9), 2854-2857 CODEN: JOCEAH; ISSN: 0022-3263

Document Type

Journal

Language

English

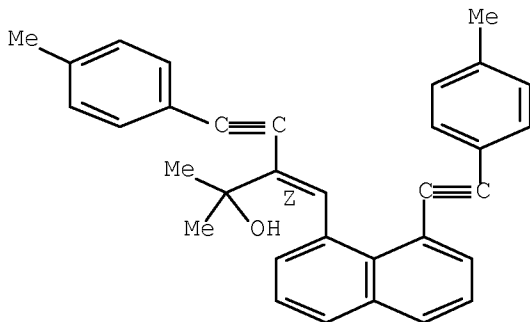
Abstract

The palladium-catalyzed insertion of 1-alkynes into internal alkynes which are bent out of linearity by the interference with a peri or ortho substituent led to enynes regioselectively. The resulting enynes undergo a new type of intramol. thermal cycloaddn., which can be used for the annulation of an aryl ring onto naphthalene derivs. to afford fluoranthenes. The cyclization of (E)-1-(1-buten-3-ynyl)-8-ethynynaphthalene could also be performed in the presence of a Cu(I) catalyst at room temperature

Hit Structure

CAS Registry Number
205124-39-6 CAPLUS

Chemical or Trade Name
4-Pentyn-2-ol, 2-methyl-5-(4-methylphenyl)-3-[[8-[2-(4-methylphenyl)ethynyl]-1-naphthalenyl]methylene]-, (3Z)- (CA INDEX NAME)



OS.CITING REF COUNT: 23 THERE ARE 23 CAPLUS RECORDS THAT CITE THIS RECORD (23 CITINGS)

L3 ANSWER 28 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1998:247633 CAPLUS [Full-text](#)

Document Number

128:295129

Title

Synthesis and characterization of well-defined fully conjugated hyperbranched oligomers of β,β -dibromo-4-ethynylstyrene

Author/Inventor

Fomina, Lioudmila; Guadarrama, Patricia; Fomine, Serguei; Salcedo, Roberto; Ogawa, Takeshi

Patent Assignee/Corporate Source

Instituto Investigaciones Materiales, Univ. Nacional Autonoma de Mexico, Mexico, 04510, Mex.

Source

Polymer (1998), 39(12), 2629-2635 CODEN: POLMAG; ISSN: 0032-3861

Document Type

Journal

Language

English

Abstract

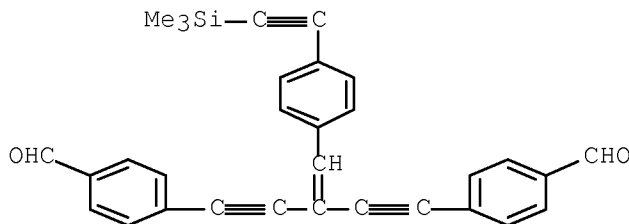
Well-defined dendritic oligomers of

poly(β,β -dibromo-4-ethynylstyrene) of the first and second generation were synthesized by a stepwise synthesis, and characterized. NMR and theor. calcs. showed that free rotation around formal single bonds is hampered by conjugation. All of the oligomers were blue emitters with their emission maxima correlating with the number of repeating units. All dendrimers except β,β -bis[β',β' -di(β'',β'' -dibromostyryl)-4'-ethynyl]styryl-4'-ethynyl]-4-ethynylstyrene showed two maxima in the excitation spectra.

Hit Structure

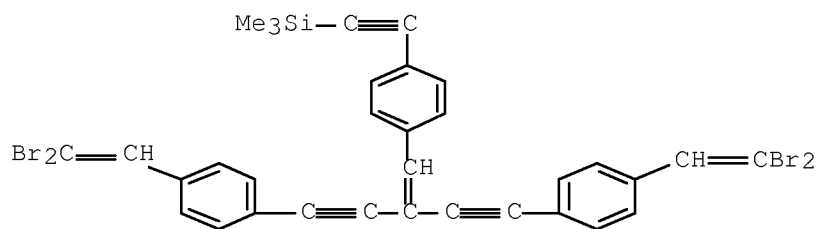
CAS Registry Number
206181-71-7 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (9CI) (CA INDEX NAME)



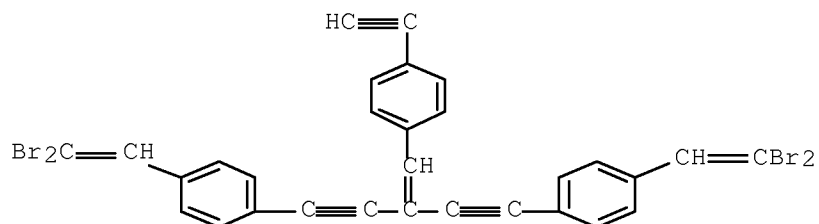
CAS Registry Number
206181-72-8 CAPLUS

Chemical or Trade Name
Silane, [[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)



CAS Registry Number
206181-73-9 CAPLUS

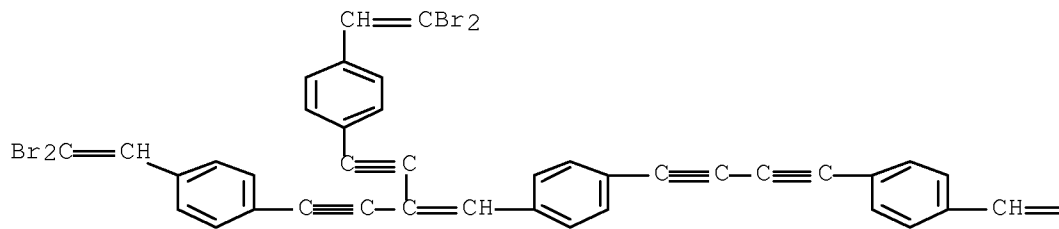
Chemical or Trade Name
Benzene, 1,1'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[4-(2,2-dibromoethenyl)- (9CI) (CA INDEX NAME)]



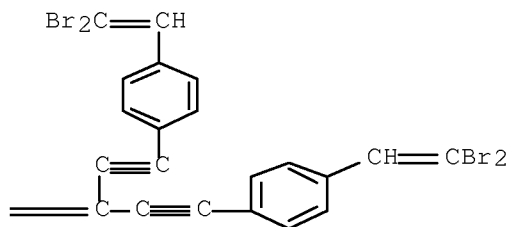
CAS Registry Number
206181-74-0 CAPLUS

Chemical or Trade Name
Benzene, 1,1'-[(1,3-butadiyne-1,4-diyl]bis[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)]

PAGE 1-A

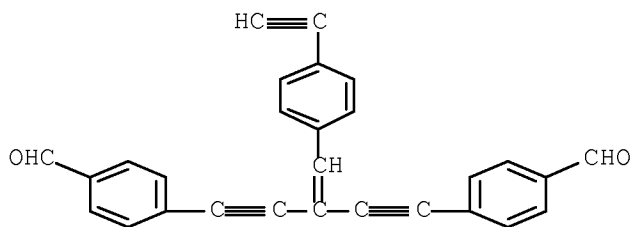


PAGE 1-B



CAS Registry Number
206181-75-1 CAPLUS

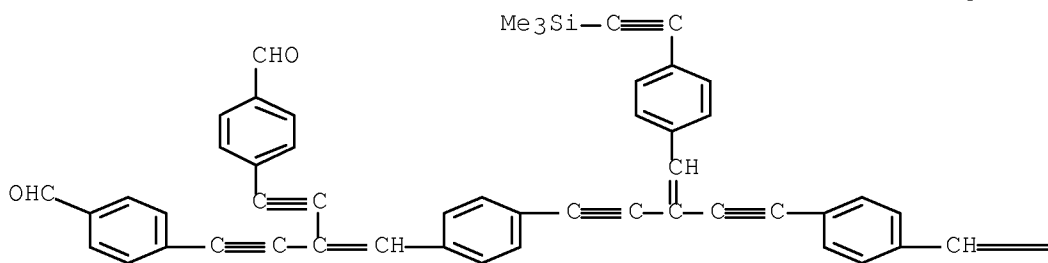
Chemical or Trade Name
Benzaldehyde, 4,4'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)]



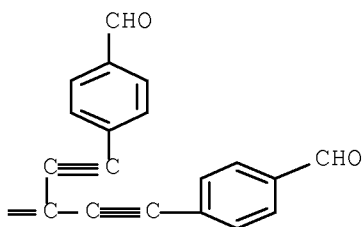
CAS Registry Number
206181-76-2 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

PAGE 1-A



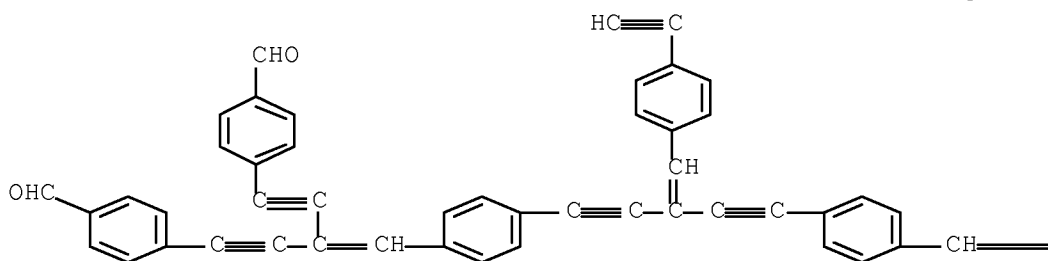
PAGE 1-B

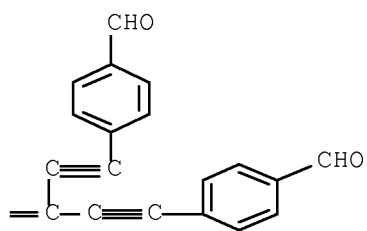


CAS Registry Number
206181-77-3 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[[3-[[4-ethynylphenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

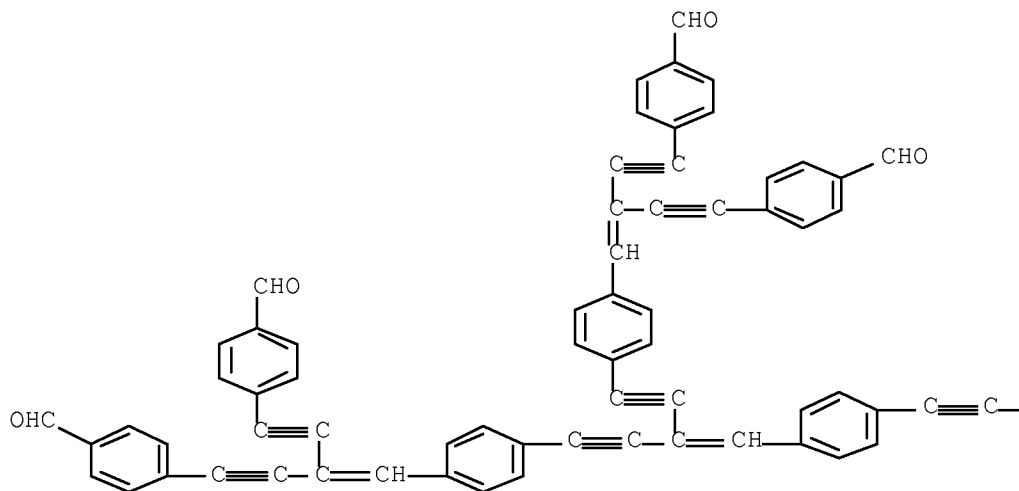
PAGE 1-A

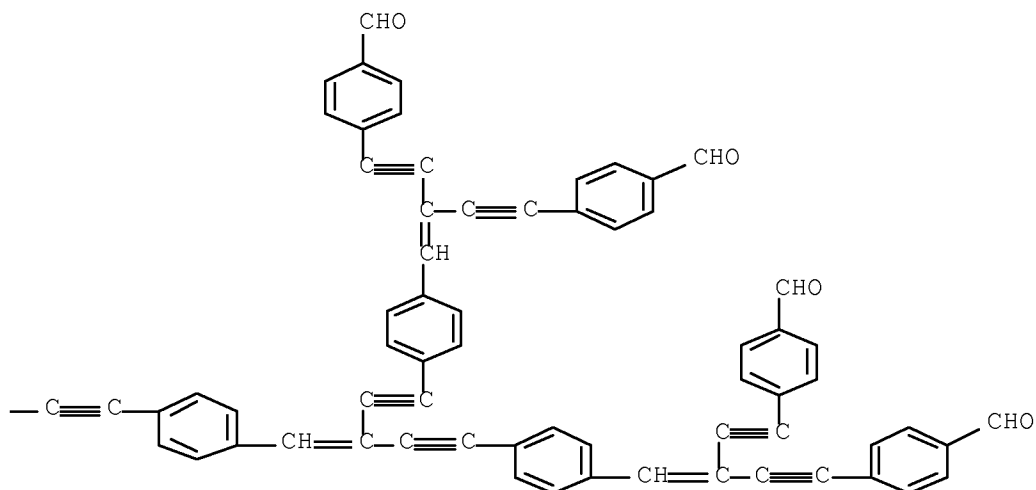




CAS Registry Number
206181-78-4 CAPLUS

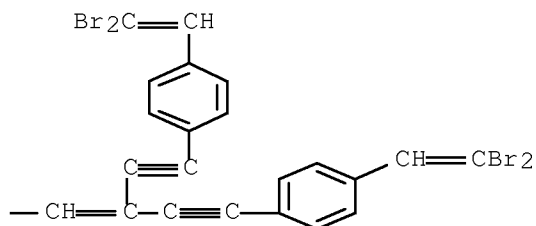
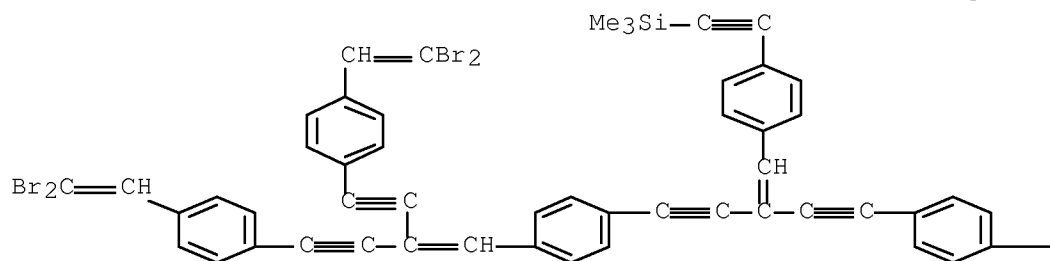
Chemical or Trade Name
Benzaldehyde, 4,4'-[1,3-butadiyne-1,4-diylbis[4,1-phenylene[3-[[4-(4-formylphenyl)-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-3-buten-1-yne-4,1-diyl]-4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)





CAS Registry Number
206181-79-5 CAPLUS

Chemical or Trade Name
Silane, [[4-[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS
RECORD (11 CITINGS)

.L3 ANSWER 29 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1996:303100 CAPLUS [Full-text](#)

Document Number

125:11582

Title

Synthesis and polymerization of β,β -dibromo-4-ethynylstyrene; preparation of a new polyconjugated, hyperbranched polymer

Author/Inventor

Fomina, Lioudmila; Salcedo, Roberto

Patent Assignee/Corporate Source

Inst. Investigaciones Materiales, Circuito Exterior, Ciudad Univ., Mexico City, 04510, Mex.

Source

Polymer (1996), 37(9), 1723-1728 CODEN: POLMAG; ISSN: 0032-3861

Document Type

Journal

Language

English

Abstract

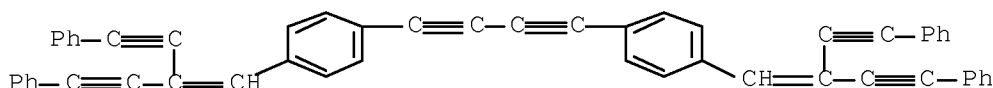
The monomer, β,β -dibromo-4-ethynylstyrene, was prepared and polymerized by the Heck reaction to give a partially soluble, conjugated hyperbranched polymer. The polymer structure was elucidated using standard spectroscopic techniques and with the aid of model compound synthesis. Theor. calcns. using the AM1 method were carried out and showed that conjugation in the polymer is partially disrupted by twisting of the benzene rings. Both the model compound and the polymer showed luminescence.

Hit Structure

CAS Registry Number
177410-40-1 CAPLUS

Chemical or Trade Name

Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-(4-phenyl-2-(phenylethynyl)-1-buten-3-ynyl)]- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)

.L3 ANSWER 30 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1995:946580 CAPLUS [Full-text](#)

Document Number

124:9540

Title

Novel polymers containing discrete conjugated units, produced by the Heck reaction

Author/Inventor

Fomine, Sergei; Fomina, Lioudmila; Florentino, Hector Quiroz; Mendez, Juan Manuel; Ogawa, Takeshi

Patent Assignee/Corporate Source

Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, Coyoacan, 04510, Mex.

Source

Polymer Journal (Tokyo) (1995), 27(11), 1085-93 CODEN: POLJBB; ISSN: 0032-3896

Document Type

Journal

Language

English

Abstract

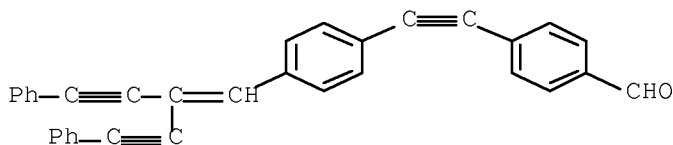
Novel monomers and polymers containing arylenevinylideneethynylene groups were synthesized via the Heck reaction. The polymers were amorphous and soluble in common organic solvents. They have T_g approx. 60°; 5% weight loss at 240-340° and undergo thermal crosslinking at 170-190° with loss of triple bonds. One of the polymers exhibits strong blue luminescence with emission maxima approx. 380-390 and 470-480 nm with excitation at 320 nm. All polymers show 3rd order NLO susceptibility approx. 10⁻¹⁰ esu.

Hit Structure

CAS Registry Number
171296-95-0 CAPLUS

Chemical or Trade Name

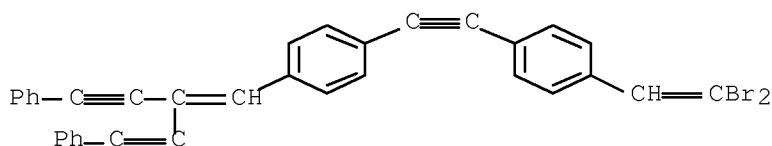
Benzaldehyde, 4-[2-[4-(2,2-dibromoethenyl)phenyl]ethynyl]-4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]phenyl]ethynyl]- (CA INDEX NAME)



CAS Registry Number
171296-96-1 CAPLUS

Chemical or Trade Name

Benzene, 1-[2-[4-(2,2-dibromoethenyl)phenyl]ethynyl]-4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)

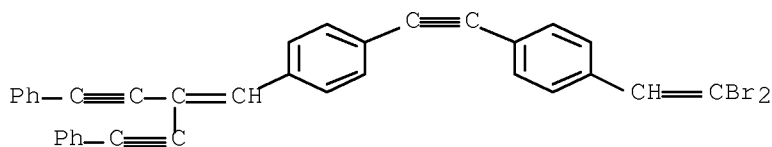


CAS Registry Number
171296-99-4 CAPLUS

Chemical or Trade Name
Decanedioic acid, di-2-propynyl ester, polymer with
1-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-4-[4-phenyl-2-(phenylethynyl)-1-
buten-3-ynyl]benzene (9CI) (CA INDEX NAME)

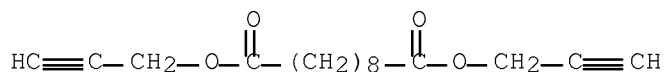
CM
1

CRN 171296-96-1
CMF C34 H20 Br2



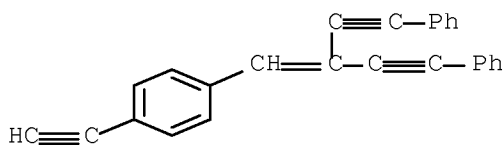
CM
2

CRN 93164-22-8
CMF C16 H22 O4



CAS Registry Number
171297-02-2 CAPLUS

Chemical or Trade Name
Benzene, 1-ethynyl-4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]-
(CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS
RECORD (11 CITINGS)

.L3 ANSWER 31 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number
1995:642218 CAPLUS [Full text](#)
Document Number
123:33763

Title
Synthesis and molten-state polymerization of some novel conjugated diacetylenes
Author/Inventor
Fomina, Lioudmila; Allier, Hector; Fomine, Sergei; Salcedo, Roberto; Ogawa, Takeshi
Patent Assignee/Corporate Source
Inst. Investigaciones Materiales, Ciudad Univ., Mexico, 04510, Mex.

Source
Polymer Journal (Tokyo) (1995), 27(6), 591-600 CODEN: POLJBJ; ISSN: 0032-3896
Document Type
Journal

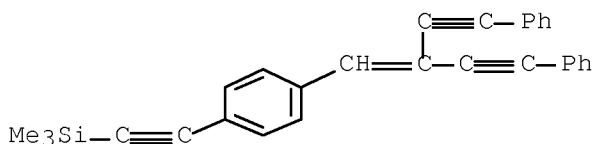
Language
English

Abstract
A series of new, highly conjugated diacetylenes, 4-ethynylstilbene derivs., was synthesized and their polymerization was studied. None of them was found to undergo topochem. polymerization in the solid state but they readily polymerized in the molten state to give red transparent and amorphous polymers. All the polymers had an absorption maximum in the visible spectra around 500 nm, and FT-IR data showed the enyne structure of the polymer chain resulted from 1,4-addition

Hit Structure

CAS Registry Number
164467-30-5 CAPLUS

Chemical or Trade Name
Benzene, 1-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]-4-[2-(
trimethylsilyl)ethynyl]- (CA INDEX NAME)

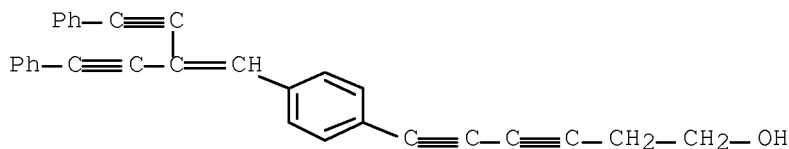


CAS Registry Number
164467-25-8 CAPLUS

Chemical or Trade Name
3,5-Hexadiyn-1-ol, 6-[4-[4-phenyl-2-(phenylethynyl)-1-buten-3-ynyl]phenyl]-
, homopolymer (9CI) (CA INDEX NAME)

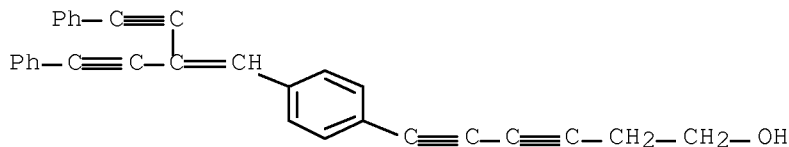
CM
1

CRN 164467-20-3
CMF C30 H20 O



CAS Registry Number
164467-20-3 CAPLUS

Chemical or Trade Name
3,5-Hexadiyn-1-ol, 6-[4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS
RECORD (11 CITINGS)

.L3 ANSWER 32 OF 32 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1994:52234 CAPLUS [Full-text](#)

Document Number

121:122234

Title

Diffuoride derivative and liquid crystal composition containing the same

Author/Inventor

Yokokoji, Osamu; Irisawa, Jun; Koh, Hidemasa

Patent Assignee/Corporate Source

Asahi Glass Co., Ltd., Japan

Source

PCT Int. Appl., 43 pp. CODEN: PIXXD2

Document Type

Patent

Language

Japanese

Patent Information

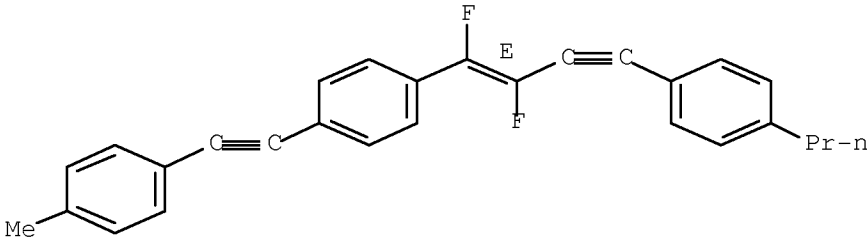
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9405613	A1	19940317	WO 1993-JP1235	19930901
EP 628528	A1	19941214	EP 1993-919602	19930901
JP 06263661	A	19940920	JP 1993-219709	19930903
JP 3564711	B2	20040915		
US 5419851	A	19950530	US 1994-211625	19940420
JP 2004292454	A	20041021	JP 2004-115211	20040409
JP 3707493	B2	20051019		

Abstract

Diffuoride derivs. represented by the general formula: R1(A1Y1)mA2CF:CF:C.tplbond.CA3(Y2A4)nR2 (A1 - A4 = trans-1,4-cyclohexylene, 1,4-cyclohexenylene, or 1,4-phenylene wherein ≥1 CH groups of each ring may be substituted by N or ≥1 CH2 groups of the ring may be substituted by O or S; m, n = 0, 1; R1, R2 = C1-10 alkyl, halo, cyano wherein (1) O, CO2, or O2C may be inserted between the C-C bond of alkyl or that between alkyl and ring, (2) a part of the C-C bonds in alkyl is replaced by C:C or C.tplbond.C bond, or (3) one CH2 group in alkyl is replaced by CO group; Y1, Y2 = CO2, O2C, C.tplbond.C, CH2CH2, CH:CH, OCH2, CH2O) are prepared. These compds. have low viscosity, are light-stable, and hence can provide a liquid crystal composition having high response speed. Thus, 0.1 mol ClCF:CF2 was blown into THF at -100° followed by adding dropwise 62.1 mL 1.61 M BuLi/hexane, stirring for 30 min, adding dropwise 0.1 mol Me3SiCl, stirring for 1 h, adding dropwise a solution of 4-propylphenyl lithium in THF (prepared from 4-propyl iodobenzene and BuLi) at -100°, and stirring for 2 h at 0° to give 75% (Z)-4-PrC6H4CF:CFSiMe3. The latter compound (0.075 mol) was reacted with 0.15 mol KF in aqueous MeCN at 70° for 1 h to give 83% (E)-4-PrC6H4CF:CFH which (0.062 mol) was dissolved in THF, cooled to -78°, and treated dropwise with 38.5 mL 1.61 M BuLi/hexane followed by stirring for 30 min, adding 15.7 g iodine, and stirring at room temperature for 4 h to give 83% (E)-4-PrC6H4CF:CFI. The latter compound (0.051 mol) and 0.051 mol 4-propylphenylacetylene were dissolved in 100 mL Et3N followed by adding Pd(PPh3)2Cl2 and CuI and the resulting mixture was allowed to react at room temperature for 6 h to give 70% diphenyldifluorobutenyne

CAS Registry Number
156869-08-8 CAPLUS

Chemical or Trade Name
Benzene, 1-[1,2-difluoro-4-(4-propylphenyl)-1-buten-3-ynyl]-4-[(4-methylphenyl)ethynyl]-, (E)- (9CI) (CA INDEX NAME)

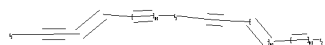


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)

=>
---Logging off of STN---

=>
Executing the logoff script...

=>



chain nodes :
1 2 3 4 5 6 7 8 9 11 15 16 17 18 19
chain bonds :
1-2 1-11 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-15 15-16 16-17 17-18 18-19
exact/norm bonds :
1-11 6-7 7-8 18-19
exact bonds :
1-2 2-3 3-4 4-5 5-6 8-9 9-15 15-16 16-17 17-18

G1:Cb,Cy,Hy

G2:C,H,Si,Cb,Cy,Hy

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:CLASS 9:CLASS 11:Atom 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS

L1 STRUCTURE UPLOADED

=> s 11 sss full
FULL SEARCH INITIATED 12:44:38 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 12030 TO ITERATE

100.0% PROCESSED 12030 ITERATIONS 106 ANSWERS
SEARCH TIME: 00.00.01

L2 106 SEA SSS FUL L1

=> s 12
L3 32 L2

=> 13 and (py<=2004 or ay<=2004)
25158915 PY<=2004
5170681 AY<=2004
L4 22 L3 AND (PY<=2004 OR AY<=2004)

=> d ibib abs hitatr 1-
YOU HAVE REQUESTED DATA FROM 22 ANSWERS - CONTINUE? Y/(N):y

.L4 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number
2004:832644 CAPLUS [Full Text](#)
Document Number
142:38113

Title
Site-Selective Monofunctionation of Dialkynylpyridines and Its Application for Preparation of Highly Fluorescent π -Conjugated Oligomers

Author/Inventor
Takayama, Yuuki; Hanazawa, Takeshi; Andou, Tomohiro; Muraoka, Kenji; Ohtani, Hiroyuki; Takahashi, Mizuki; Sato, Fumie
Patent Assignee/Corporate Source
Department of Biomolecular Engineering, Tokyo Institute of Technology, Midori-ku, Yokohama, Kanagawa, 226-8501, Japan

Source
Organic Letters (2004), 6(23), 4253-4256 CODEN: ORLEF7; ISSN: 1523-7060

Document Type
Journal

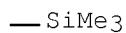
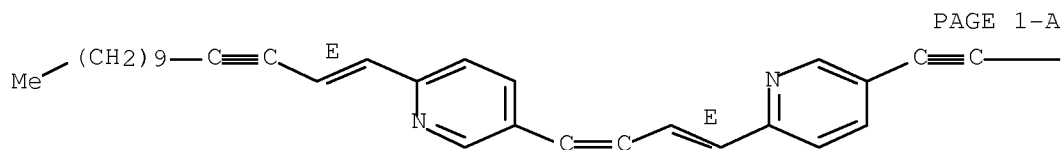
Language
English

Abstract
Reaction of Ti(O-*i*-Pr)₄/2*i*-PrMgCl reagent with 2,*n*-bis(trimethylsilyl)ethynylpyridines, where *n* is 3, 4, 5, and 6, or with 3,4-bis(trimethylsilyl)ethynylpyridines, proceeded with excellent site-selectivity to afford the corresponding monofunctionated complex. Synthetic application of the reaction was demonstrated by an efficient preparation of π -conjugated oligomers having pyridine and enyne units alternately, which possess intense blue fluorescence emission. Thus, reaction of 2,3-bis(trimethylsilyl)ethynylpyridine with Ti(O-*i*-Pr)₄/2*i*-PrMgCl reagent in Et₂O gave 84% (Z)-2-[2-(trimethylsilyl)ethenyl]-3-[(trimethylsilyl)ethynyl]pyridine.

Hit Structure

CAS Registry Number
805240-17-9 CAPLUS

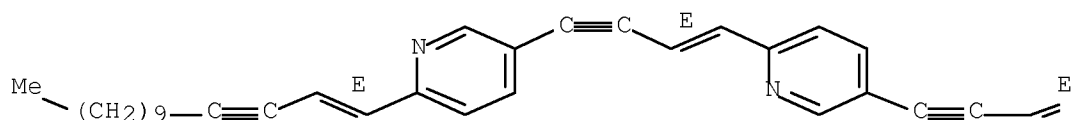
Chemical or Trade Name
Pyridine, 2-[(1E)-4-[6-(1E)-1-tetradecen-3-yn-1-yl-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)



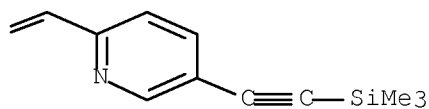
PAGE 1-B

CAS Registry Number
805240-18-0 CAPLUS

Chemical or Trade Name
Fyridine, 2-[(1E)-4-[6-[(1E)-4-[6-(1E)-1-tetradecen-3-yn-1-yl-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)



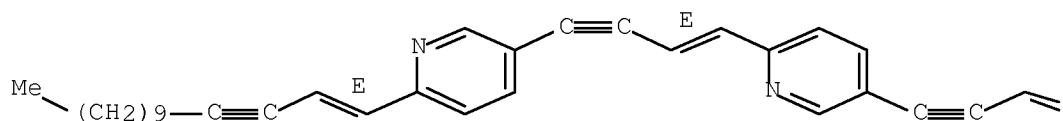
PAGE 1-B



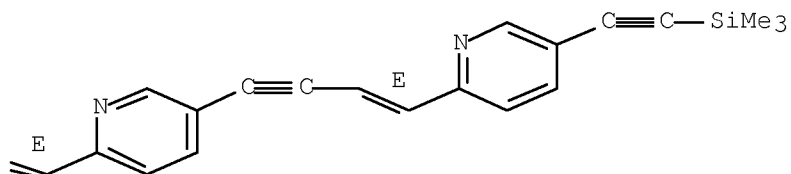
CAS Registry Number
805240-19-1 CAPLUS

Chemical or Trade Name
Fyridine, 2-[(1E)-4-[6-[(1E)-4-[6-(1E)-1-tetradecen-3-yn-1-yl-3-pyridinyl]-1-buten-3-yn-1-yl]-3-pyridinyl]-1-buten-3-yn-1-yl]-5-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

.L4 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2004:566840 CAPLUS ~~Fid:18~~

Document Number

141:261152

Title

π -Conjugated Dendrimers Based on Bis(enediynyl)benzene Units

Author/Inventor

Hwang, Gil Tae; Kim, Byeang Hyeon

Patent Assignee/Corporate Source

National Research Laboratory, Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

Source

Organic Letters (2004), 6(16), 2669-2672 CODEN: ORLEF7; ISSN: 1523-7060

Document Type

Journal

Language

English

Abstract

We have synthesized a new family of π -conjugated dendrimers that are based on bis(enediynyl)benzene units by using both divergent and convergent approaches. The compds. at all three generations have strong bluish-green fluorescence, especially the third-generation dendrimer, which has the highest extinction coefficient and quantum efficiency in this series.

Hit Structure

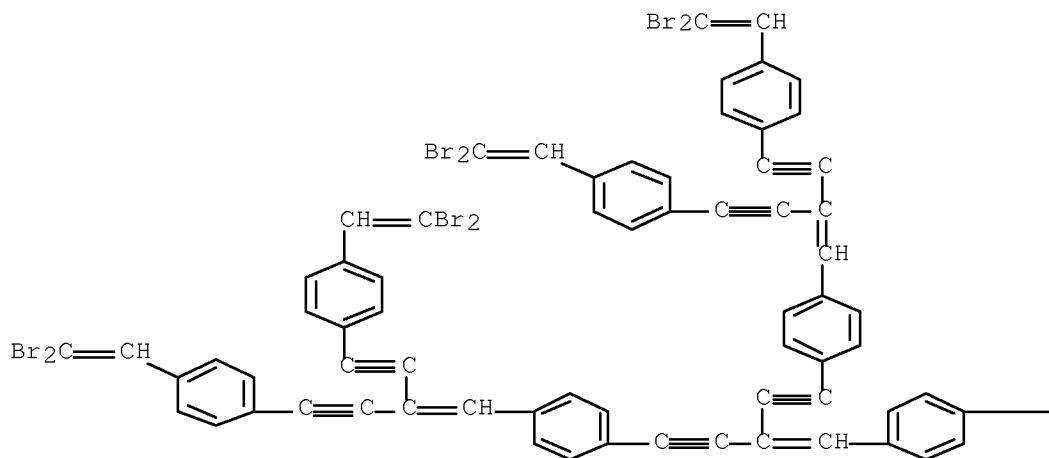
CAS Registry Number

754233-16-4 CAPLUS

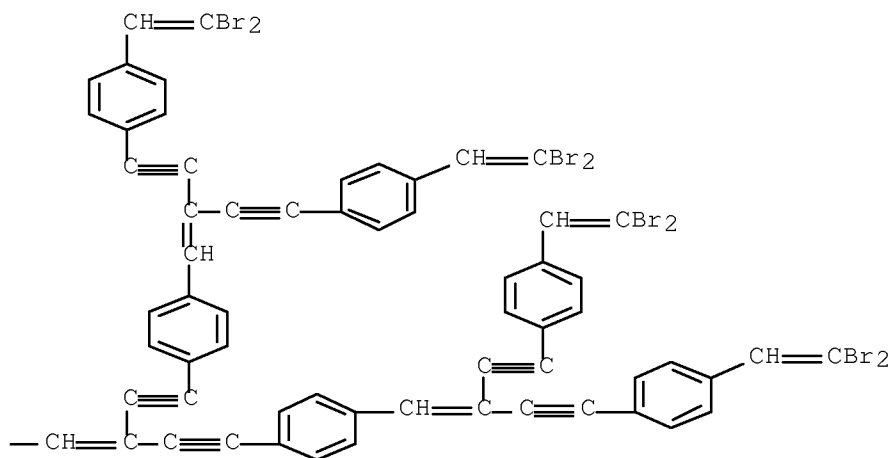
Chemical or Trade Name

Benzene, 1,4-bis[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



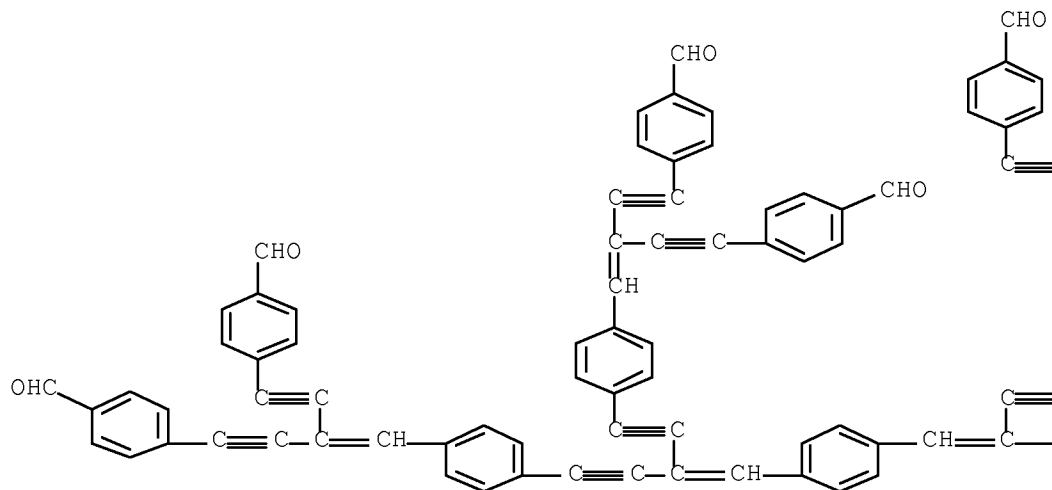
PAGE 1-B



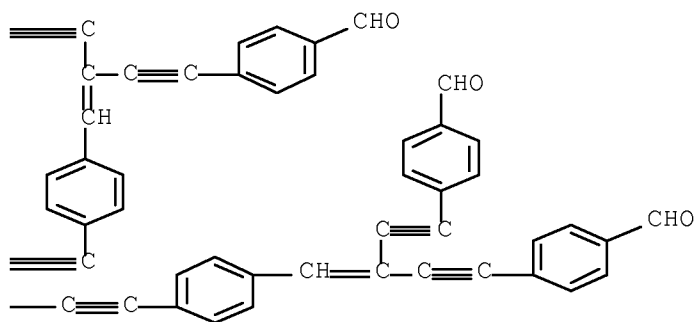
CAS Registry Number
754233-18-6 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[[3-[[4-[[4-[[4-(4-formylphenyl)-2-[[4-formylphenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[[4-(4-formylphenyl)-2-[[4-formylphenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[[4-formylphenyl]ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)

PAGE 1-A

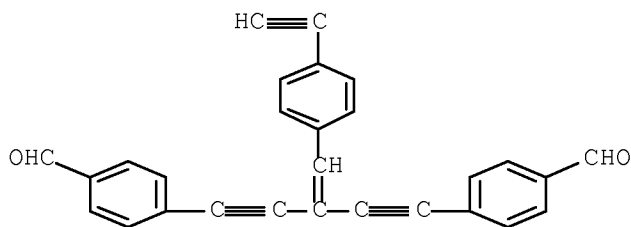


PAGE 1-B



CAS Registry Number
206181-75-1 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[3-[[4-ethynylphenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS RECORD (17 CITINGS)

. L4 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2004:480115 CAPLUS [Full-text](#)

Document Number

141:190674

Title

Synthesis of Conjugated Oligomers Having Aromatic and Enediyne Units Alternately in the Backbone that Show Intense Fluorescence Emission

Author/Inventor

Nakano, Yuuki; Ishizuka, Kenichi; Muraoka, Kenji; Ohtani, Hiroyuki; Takayama, Yuuki; Sato, Fumie

Patent Assignee/Corporate Source

Department of Biomolecular Engineering, Tokyo Institute of Technology, Midori, Yokohama, Kanagawa, 226-8501, Japan

Source

Organic Letters (2004), 6(14), 2373-2376 CODEN: ORLEF7; ISSN: 1523-7060

Document Type

Journal

Language

English

Abstract

Synthesis and fluorescence properties of *n*-conjugated compds. I (*n* = 1 - 3; X = 1,4-phenylene, 2,5-pyridine, 2,5-thiophene; R = *n*-Pr, *n*-Bu) having alternately an aromatic or heteroarom. ring and an enediyne unit in the backbone are described.

Hit Structure

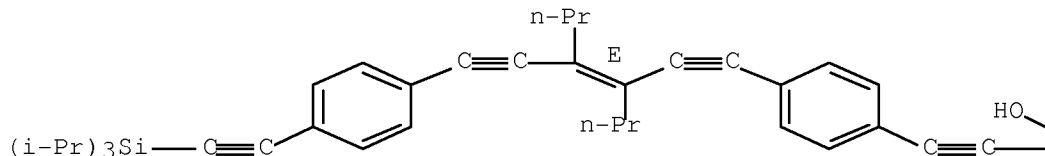
CAS Registry Number

740810-61-1 CAPLUS

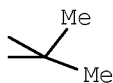
Chemical or Trade Name

3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[2-[4-[2-[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



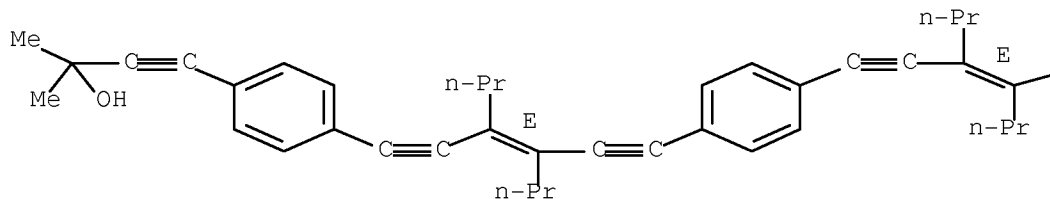
CAS Registry Number

740810-62-2 CAPLUS

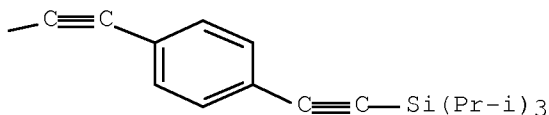
Chemical or Trade Name

3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[[4-[[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

PAGE 1-A



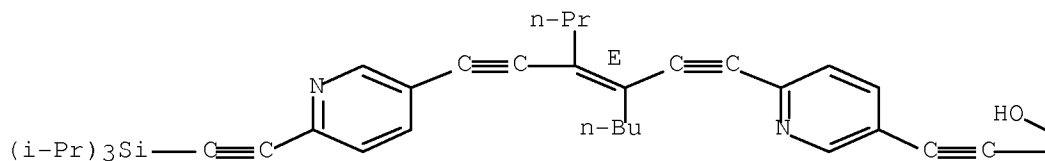
PAGE 1-B



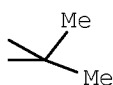
CAS Registry Number
740810-64-4 CAPLUS

Chemical or Trade Name
3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

PAGE 1-A



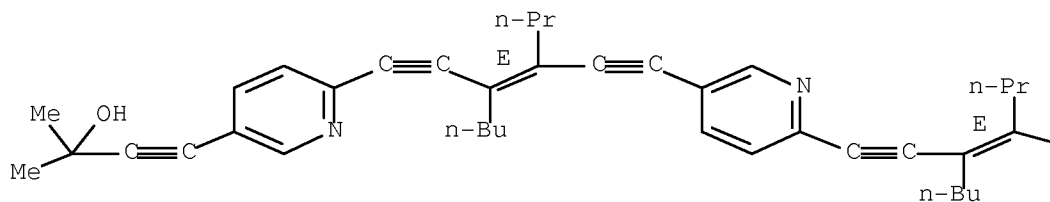
PAGE 1-B



CAS Registry Number
740810-65-5 CAPLUS

Chemical or Trade Name
3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[2-[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

PAGE 1-A



Chemical or Trade Name
3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Chemical or Trade Name
3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[5-[5-[(3E)-3-propyl-4-[5-
[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-
2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

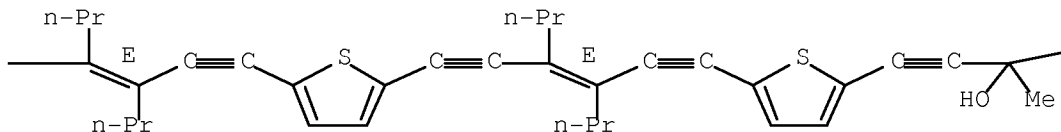
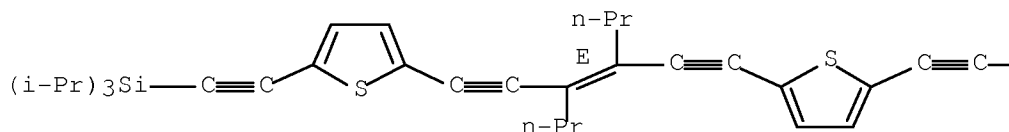
Chemical or Trade Name
3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[[4-[(3E)-3-propyl-4-[[4-
[(3E)-3-propyl-4-[[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-
hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-
hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

Chemical or Trade Name
3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)



CAS Registry Number
740810-69-9 CAPLUS

Chemical or Trade Name
3-Butyn-2-ol, 4-[5-[(3E)-4-[2-[5-[(3E)-5-ethyl-4-[2-[5-[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 23 THERE ARE 23 CAPLUS RECORDS THAT CITE THIS RECORD (24 CITINGS)

L4 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2004:38299 CAPLUS [Full-text](#)

Document Number

141:88772

Title

Electrochemical and theoretical study of a family of fully conjugated dendritic oligomers

Author/Inventor

Osorio, Gabriela; Frontana, Carlos; Guadarrama, Patricia; Frontana-Urbe, Bernardo A.

Patent Assignee/Corporate Source

Instituto de Química, UNAM, Circuito Exterior Ciudad Universitaria, Mexico, 04510, Mex.

Source

Journal of Physical Organic Chemistry (2004), 17(5), 439-447 CODEN: JPOCEE; ISSN: 0894-3230

Document Type

Journal

Language

English

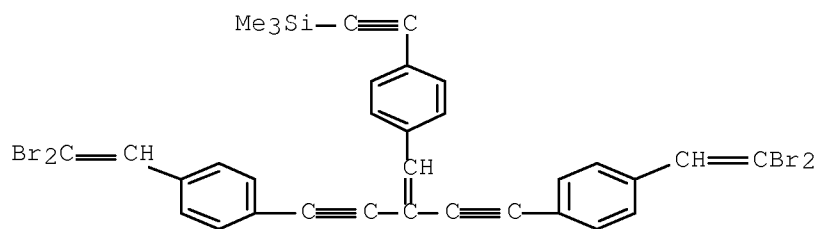
Abstract

Novel dendritic oligomers of β,β -dibromo-4-ethynylstyrene and formyl-4-ethynylstyrene were electrochem. and theor. studied to gain a better insight into their redox behavior. Correlations between calculated ionization and exptl. oxidation potentials (anodic peak potentials) were established. The best correlation was obtained when two important effects are considered in the theor. calcs., probing their strong influence: (a) structural re- accommodation in the formed radical cation and (b) solvation effects. The effect of dendritic terminal groups (dibromovinyl and formyl groups) was also analyzed. A different redox behavior was observed for these two terminal groups, presumably due to a difference in their oxidation mechanisms. A global chemical transformation for the oxidation of dibromovinyl-terminated oligomers was proposed, providing a satisfactory explanation of the electrochem. behavior within this family of (presence of adsorptive phenomena). Taking these results into account, it is possible to explain how the cation-radical species formed in these conjugated dendritic oligomers behave when cyclic voltammetry technique is applied.

Hit Structure

CAS Registry Number
716327-89-8 CAPLUS

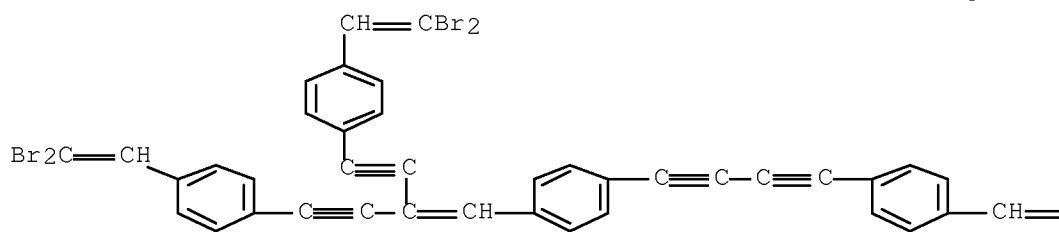
Chemical or Trade Name
Silane, [[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-, radical ion(1+) (9CI) (CA INDEX NAME)



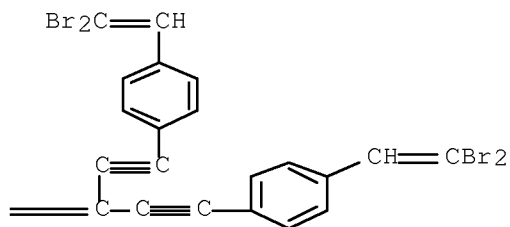
CAS Registry Number
716327-90-1 CAPLUS

Chemical or Trade Name
Benzene, 1,1'-[1,3-butadiyne-1,4-diyl]bis[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]-, radical ion(1+) (9CI) (CA INDEX NAME)

PAGE 1-A



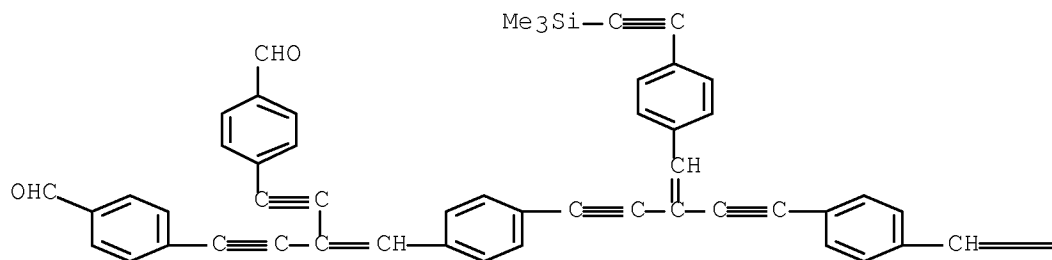
PAGE 1-B

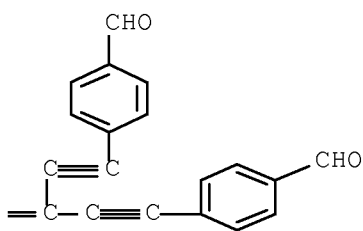


CAS Registry Number
716327-91-2 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[[4-formylphenyl]ethynyl]-3-buten-1-yne-4,1-diyl]]]bis-, radical ion(1+) (9CI) (CA INDEX NAME)

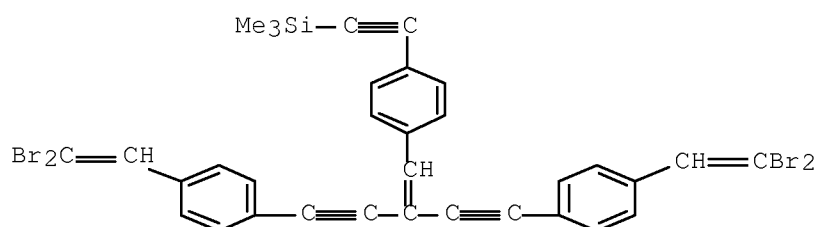
PAGE 1-A





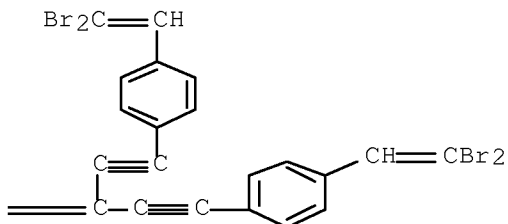
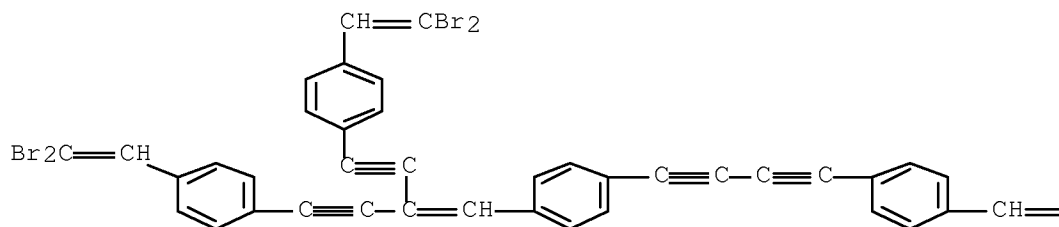
CAS Registry Number
206181-72-8 CAPLUS

Chemical or Trade Name
Silane, [[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-
(9CI) (CA INDEX NAME)



CAS Registry Number
206181-74-0 CAPLUS

Chemical or Trade Name
Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

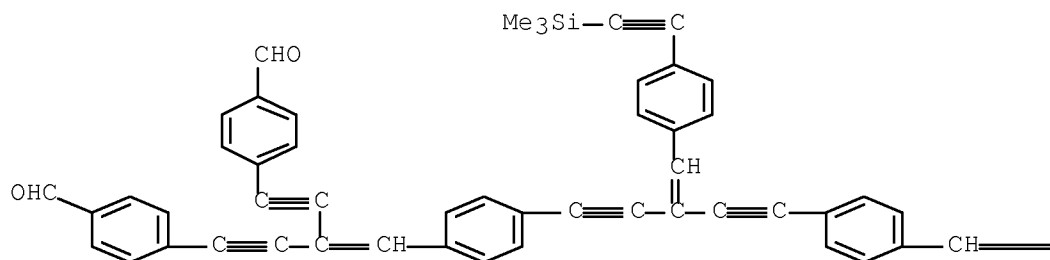


CAS Registry Number
206181-76-2 CAPLUS

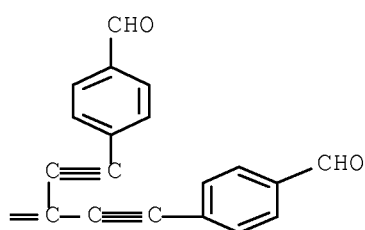
Chemical or Trade Name
Benzaldehyde, 4,4'-[[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[[4-formylphenyl]ethynyl]-3-buten-
(9CI) (CA INDEX NAME)

1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)

PAGE 1-A

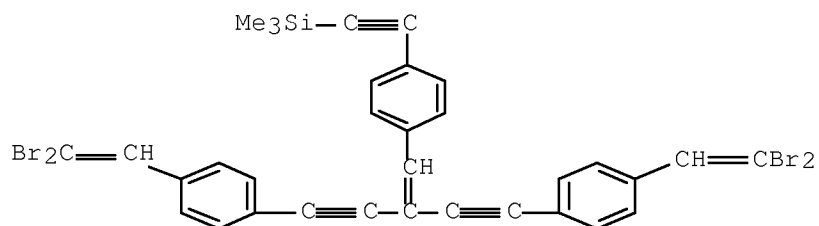


PAGE 1-B



CAS Registry Number
717144-23-5 CAPLUS

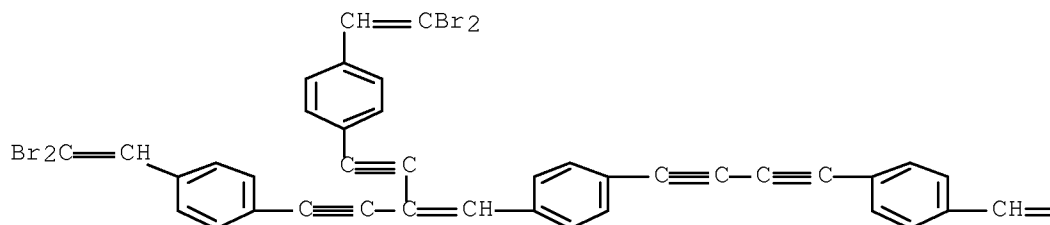
Chemical or Trade Name
Silane, [[4-[4-[4-(2,2-dibromoethyl)phenyl]-2-[4-(2,2-dibromoethyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-, radical ion(1-) (9CI) (CA INDEX NAME)

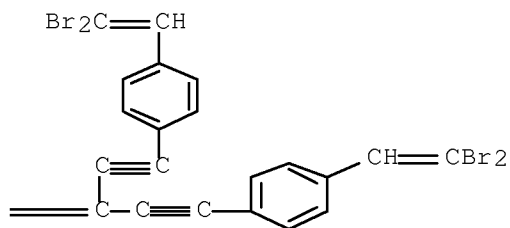


CAS Registry Number
717144-24-6 CAPLUS

Chemical or Trade Name
Benzene, 1,1'-(1,3-butadienyl-1,4-diyl)bis[4-{4-[4-(2,2-dibromoethenyl)phenyl]phenyl}ethynyl]-1-buten-3-ynyl-, radical ion(1-) (9CI) (CA INDEX NAME)

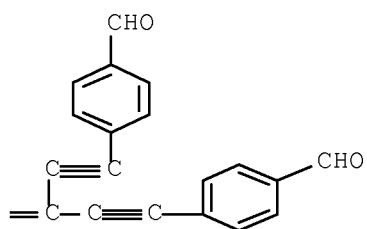
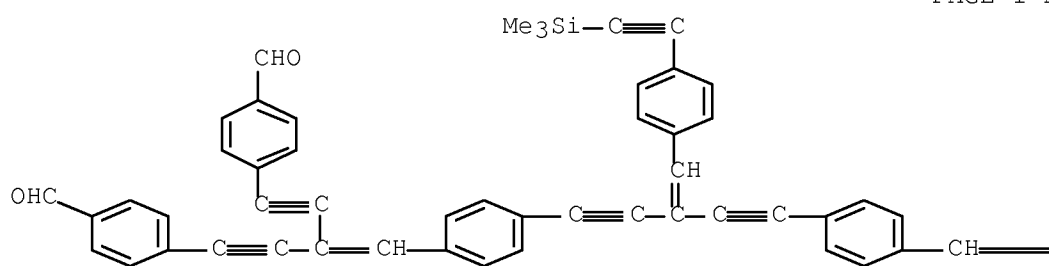
PAGE 1-A





CAS Registry Number
717144-25-7 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis-, radical ion(1-) (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

Accession Number

2004:328526 CAPLUS [Full-text](#)

Document Number

141:54000

Title

Solid-phase synthesis of oligo(triacetylene)s and oligo(phenylene triacetylene)s employing Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions

Author/Inventor

Utesch, Nils F.; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice

Patent Assignee/Corporate Source

Laboratorium fuer Organische Chemie, ETH-Hoenggerberg, HCI, Zurich, CH-8093, Switz.

Source

Helvetica Chimica Acta (2004), 87(3), 698-718 CODEN: HCACAV; ISSN: 0018-019X

Document Type

Journal

Language

English

Abstract

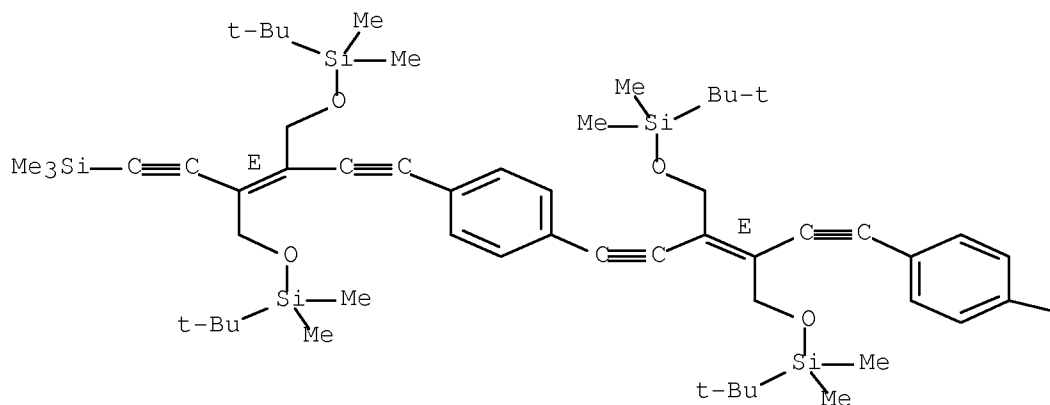
The polymer-supported synthesis of poly(triacetylene)-derived monodisperse oligomers is described, using Pd0-catalyzed Sonogashira and Cadiot-Chodkiewicz-type cross-couplings as the key steps in the construction of the acetylenic scaffolds. Merrifield resin functionalized with a 1-(4-iodoaryl)triazene linker was chosen as the polymeric support. The linker selection was made based on the results of several model studies in the liquid phase. For the solid-support synthesis of p-[C6H4C.tpbond.CC(CH2OSiMe2CMe3);C(CH2OSiMe2CMe3)C.tpbond.C]nSiMe3 [I, n = 2-4] a set of only three reactions was required: (i) Pd0-catalyzed Sonogashira cross-coupling, (ii) Me3Si-alkyne deprotection by protodesilylation, and (iii) cleavage of the linker with liberation of I. The longest-wavelength absorption maxima of I [n = 1-4] shift bathochromically with increasing oligomeric length, from λ_{max} 337 nm (I, n = 1) to 384 nm (I, n = 4). Based on the electronic absorption data, the effective conjugation length (ECL) of the oligo(phenylene triacetylene)s is estimated to involve at least four monomer units and 40 C-atoms. π -Electron conjugation in these oligomers is less efficient than in Me3Si[C6H4C.tpbond.CC(CH2OSiMe2CMe3);C(CH2OSiMe2CMe3)C.tpbond.C]nSiMe3 (II) due to poor transmittance of π -electron delocalization by the Ph rings inserted into the oligomeric backbone. Similar conclusions were drawn from the electrochem. properties of the two oligomeric series as determined by cyclic (CV) and rotating-disk voltammetry. In sharp contrast to II, I are strongly fluorescent, with the highest quantum yield Φ_F = 0.69 measured for I [n = 3]. Whereas the Sonogashira cross-coupling on solid support proceeded smoothly, optimal conditions for alkyne-alkyne cross-coupling reactions employing Pd0-catalyzed Cadiot-Chodkiewicz conditions still remain to be developed.

Hit Structure

CAS Registry Number
554459-62-0 CAPLUS

Chemical or Trade Name

4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[[[trimethylsilyl]ethynyl]-, (6E)- (9CI) (CA INDEX NAME)



PAGE 1-A

PAGE 1-B

I

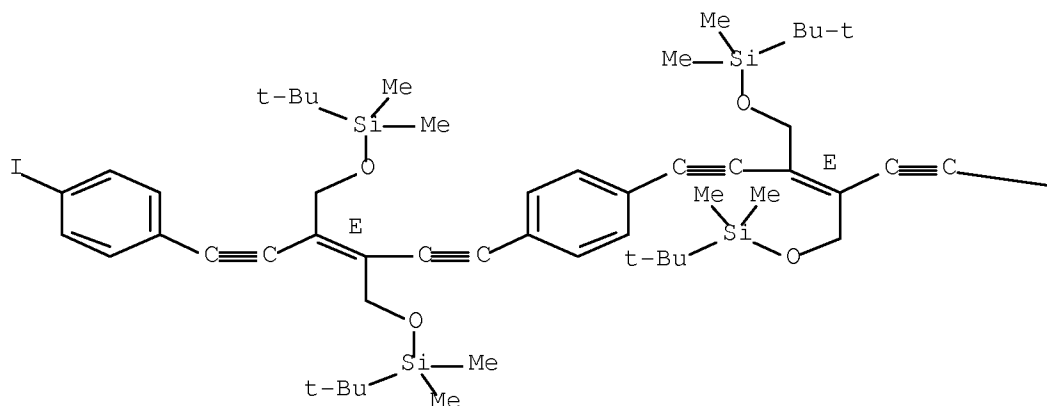
CAS Registry Number
554459-63-1 CAPLUS

Chemical or Trade Name

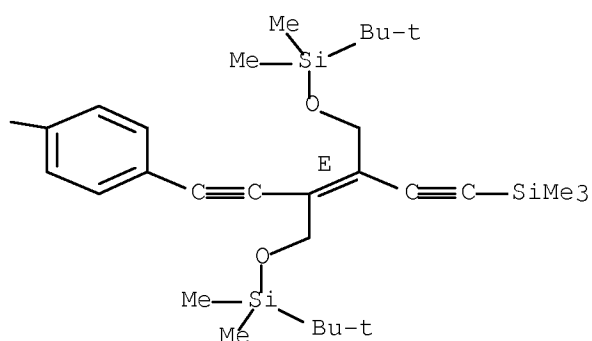
4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[[4-[(3E)-6-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-

[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

PAGE 1-A



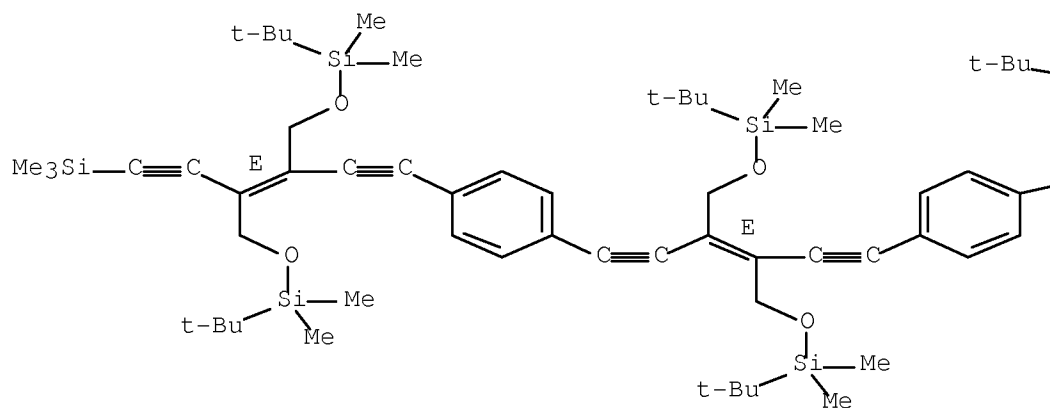
PAGE 1-B



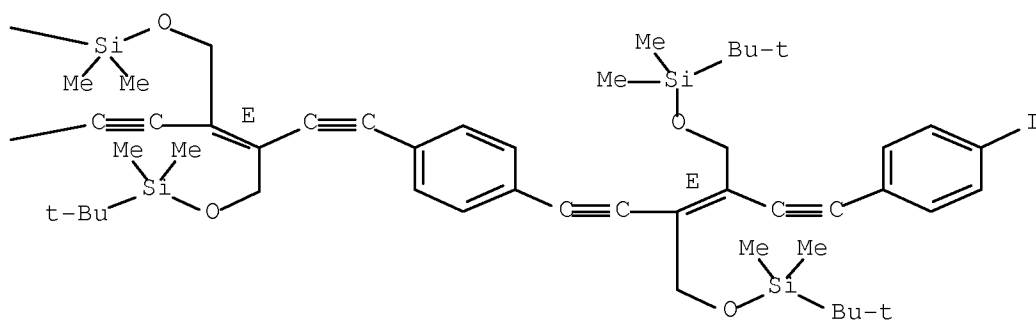
CAS Registry Number
554459-64-2 CAPLUS

Chemical or Trade Name
4,9-Dioxo-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)

PAGE 1-A



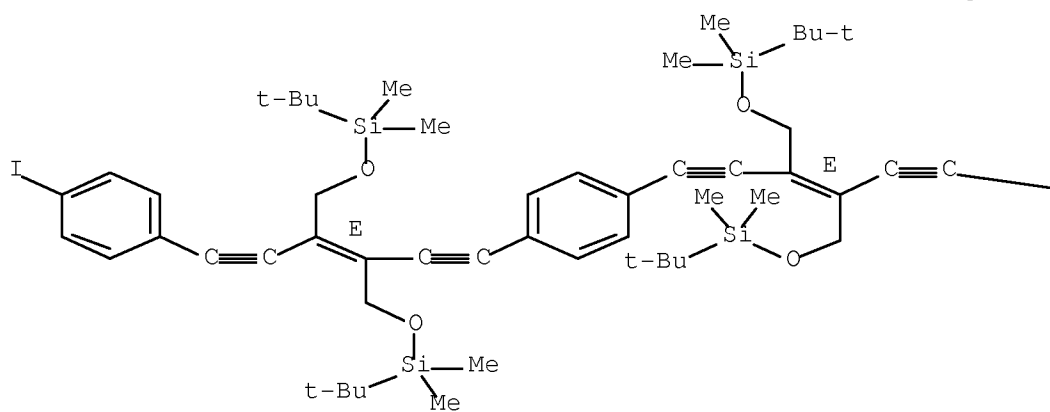
PAGE 1-B

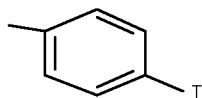


CAS Registry Number
704916-29-0 CAPLUS

Chemical or Trade Name
4,9-Dioxo-3,10-disiladodec-6-ene, 6,6'-(1,4-phenylenedi-2,1-ethynediyl)bis[7-[(4-iodophenyl)ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E,6'E)- (9CI) (CA INDEX NAME)

PAGE 1-A





OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD
(8 CITINGS)

.L4 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2003:491916 CAPLUS ~~Fulltext~~

Document Number

139:395637

Title

Synthesis of differentially protected/functionalised acetylenic building blocks from p-benzoquinone and their use in the synthesis of new enediynes

Author/Inventor

Sankararaman, Sethuraman, Srinivasan, Manivannan

Patent Assignee/Corporate Source

Department of Chemistry, Indian Institute of Technology Madras, Madras, 600 036, India

Source

Organic & Biomolecular Chemistry (2003), 1(13), 2388-2392 CODEN: OBCRAK; ISSN: 1477-0520

Document Type

Journal

Language

English

Abstract

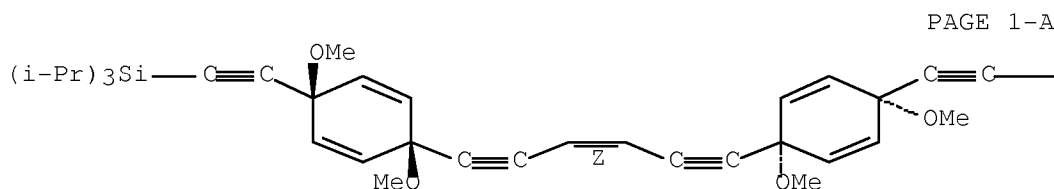
Sequential addition of two different lithium acetylides to p-benzoquinone yielded diastereomeric mixts. of 1,4-diethynylcyclohexa-2,5-diene-1,4-diols I [R = (Me₂CH)₃Si, (EtO)₂CH] with different protective/functional groups on the two ethynyl groups. Selective monodeprotection of the di-Me ethers of I to the corresponding terminal acetylenes followed by Pd(0)-mediated coupling with (Z)-1,2-dichloroethene yielded new enediynes II bearing cyclohexa-2,5-diene units.

Hit Structure

CAS Registry Number
626235-20-9 CAPLUS

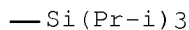
Chemical or Trade Name

Silane, [(3Z)-3-hexene-1,5-diyne-1,6-diylbis[(cis-1,4-dimethoxy-2,5-cyclohexadiene-1,4-diyl)-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)



PAGE 1-A

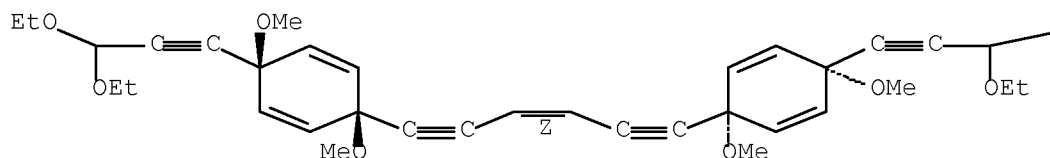
PAGE 1-B



CAS Registry Number
626235-21-0 CAPLUS

Chemical or Trade Name

1,4-Cyclohexadiene, 3,3'-(3Z)-3-hexene-1,5-diyne-1,6-diylbis[6-(3,3-diethoxy-1-propynyl)-3,6-dimethoxy-, (cis,cis)- (9CI) (CA INDEX NAME)

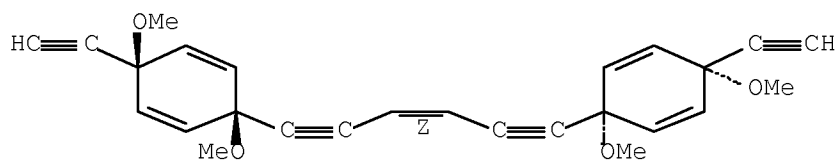


PAGE 1-A



CAS Registry Number
626235-22-1 CAPLUS

Chemical or Trade Name
1,4-Cyclohexadiene, 3,3'-(3Z)-3-hexene-1,5-diyne-1,6-diylbis[6-ethynyl-3,6-dimethoxy-, (cis,cis)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
(6 CITINGS)

L4 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2003:234291 CAPLUS [Fulltext](#)

Document Number

139:85055

Title

Acetylenic scaffolding on solid support: Poly(triacetylene)-derived oligomers by Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions

Author/Inventor

Utesch, Nils F.; Diederich, Francois

Patent Assignee/Corporate Source

Laboratorium für Organische Chemie, ETH-Honggerberg, HCI, Zurich, CH-8093, Switz.

Source

Organic & Biomolecular Chemistry (2003), 1(2), 237-239 CODEN: OBCRAK; ISSN: 1477-0520

Document Type

Journal

Language

English

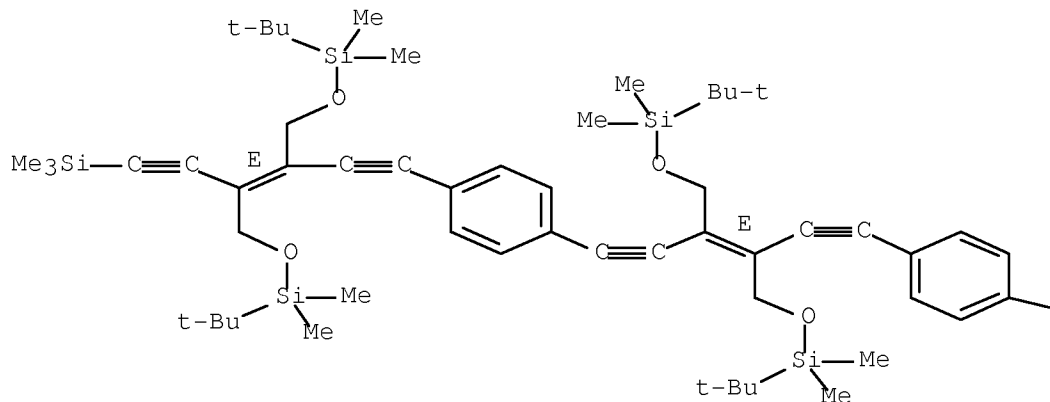
Abstract

Synthesis of poly(triacetylene)-derived oligomers by Pd(0)-catalyzed Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions on solid support is reported. Oligo(phenylene triacetylene)s, e.g., [[4-C6H4C.tpbond.CCR.CRC.tpbond.C]nSiMe3 (R = CH2OSiButMe2, n = 1, 2, 3, 4) members of a new class of linearly π -conjugated oligomers with all-C backbones, feature very high fluorescence intensities.

Hit Structure

CAS Registry Number
554459-62-0 CAPLUS

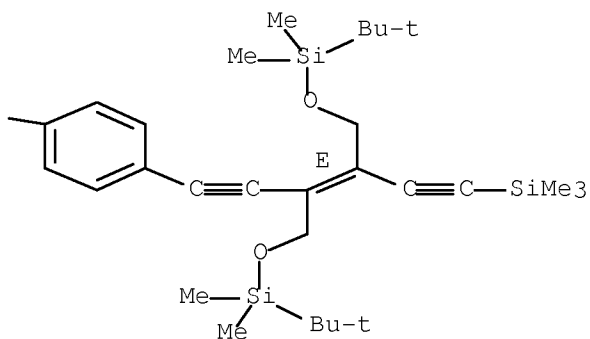
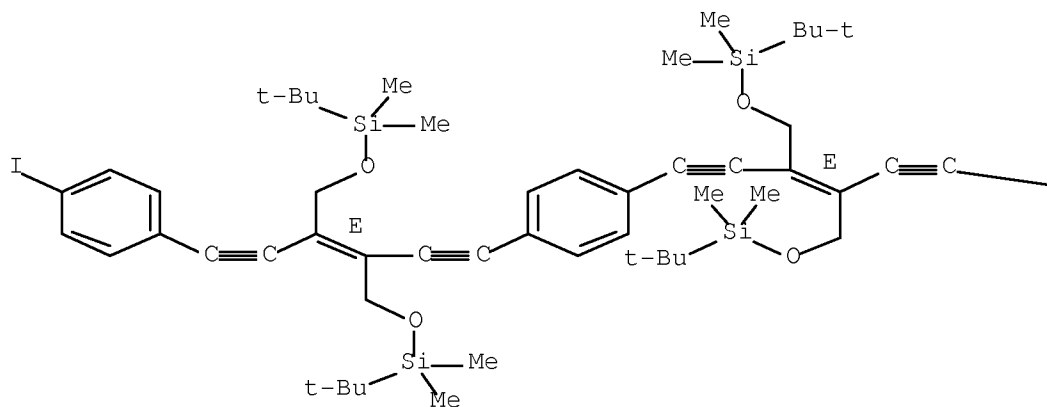
Chemical or Trade Name
4,9-Dioxo-3,10-disiladodec-6-ene, 6-[[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[[trimethylsilyl]ethynyl]-, (6E)- (9CI) (CA INDEX NAME)



I

CAS Registry Number
554459-63-1 CAPLUS

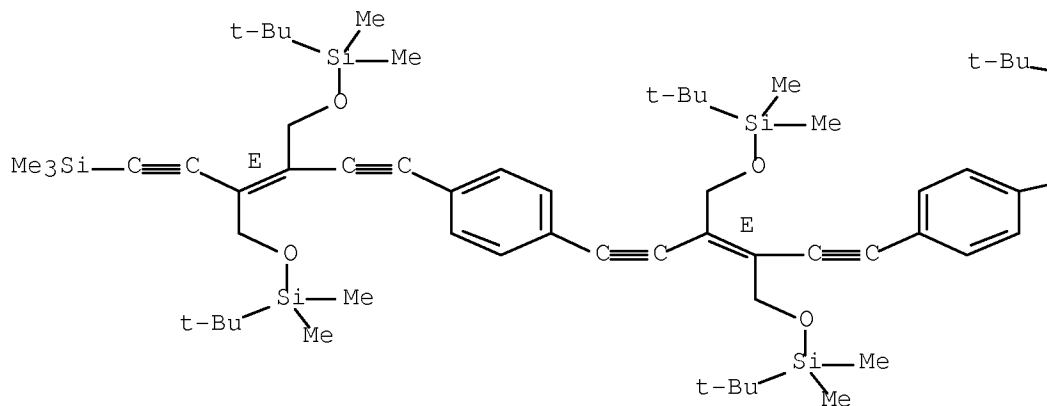
Chemical or Trade Name
4,9-Dioxa-3,10-disiladodec-6-ene, 6-[[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[[trimethylsilyl]ethynyl]-, (6E)- (9CI) (CA INDEX NAME)



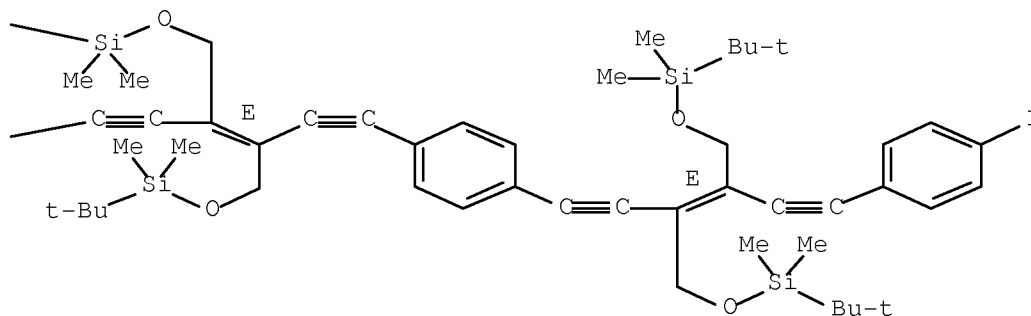
CAS Registry Number

Chemical or Trade Name
 4,9-Dioxo-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)

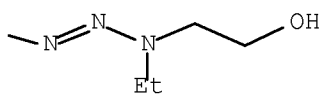
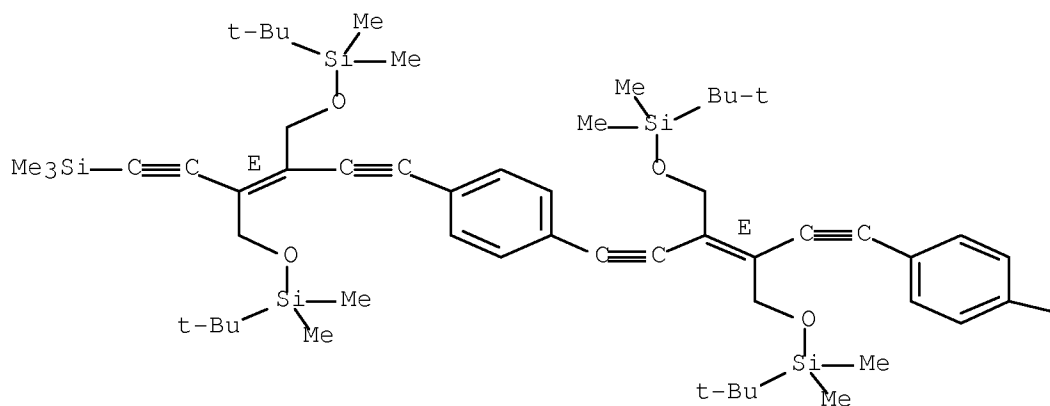
PAGE 1-A



PAGE 1-B



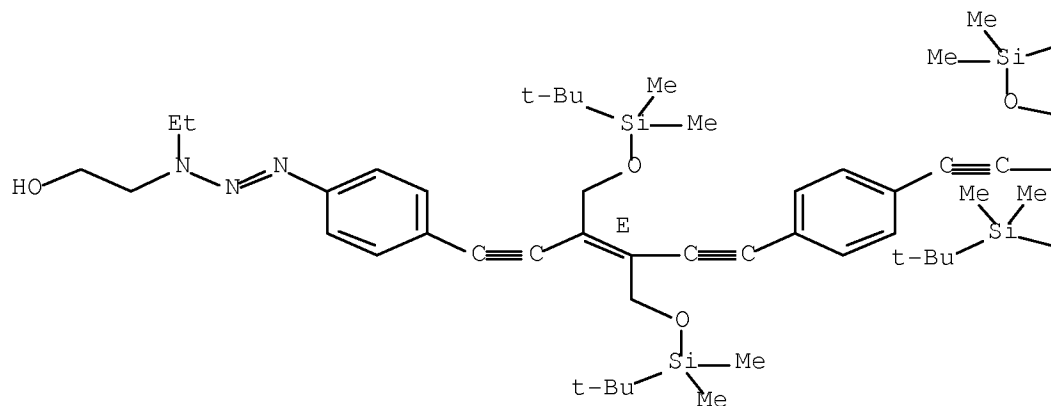
Chemical or Trade Name
 Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazene-1-yl]- (CA INDEX NAME)



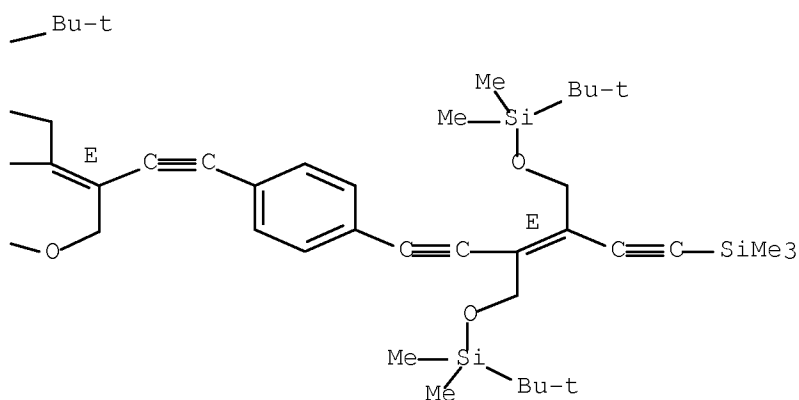
CAS Registry Number
554459-72-2 CAPLUS

Chemical or Trade Name
Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazen-1-yl]- (CA INDEX NAME)

PAGE 1-A



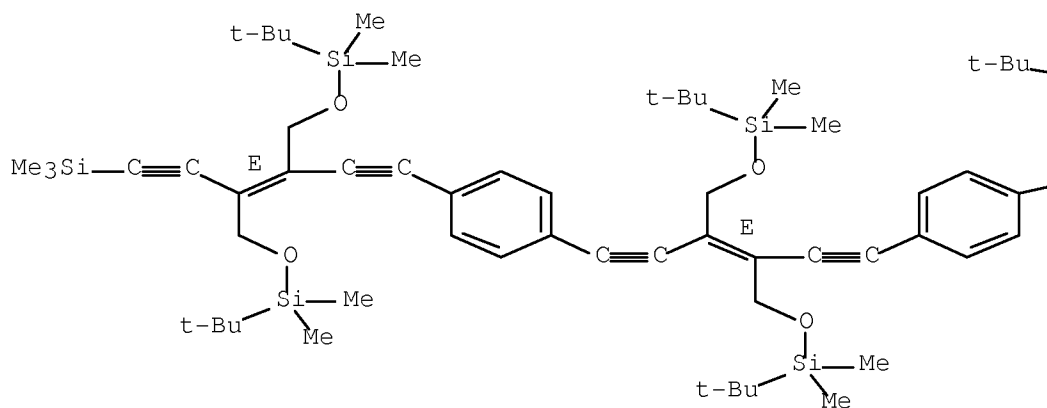
PAGE 1-B



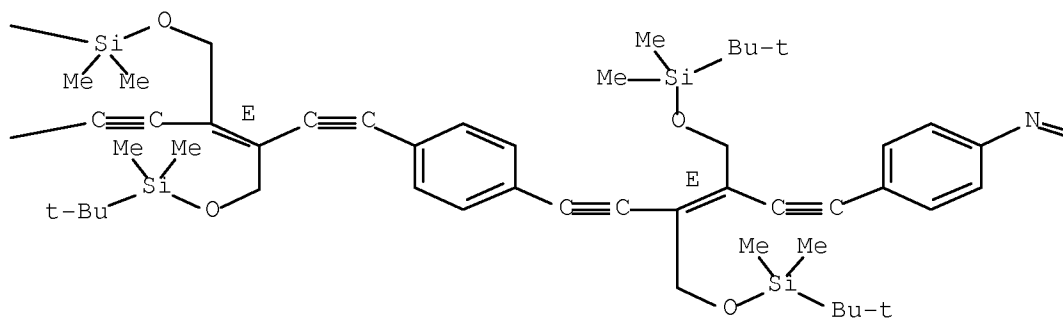
CAS Registry Number
554459-73-3 CAPLUS

Chemical or Trade Name
Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazene-1-yl]- (CA INDEX NAME)

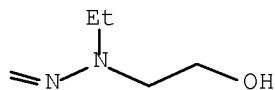
PAGE 1-A



PAGE 1-B



PAGE 1-C



OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (19 CITINGS)

, L4 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2002:658690 CAPLUS [Full-text](#)

Document Number

137:208374

Title

Manufacturing method of semiconductor device using mask pattern having high etching resistance

Author/Inventor

Ohuchi, Junko; Sato, Yasuhiko; Shiobara, Eishi; Hayashi, Hisataka; Ohiwa, Tokuhisa; Onishi, Yasunobu

Patent Assignee/Corporate Source

Kabushiki Kaisha Toshiba, Japan

Source

U.S. Pat. Appl. Publ., 26 pp. CODEN: USXXCO

Document Type

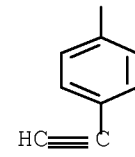
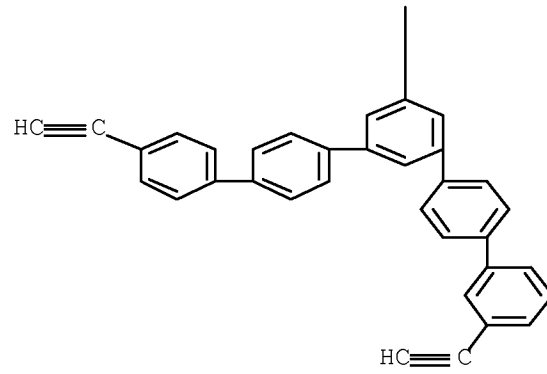
Patent

Language

English

Patent Information

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
------------	------	------	-----------------	------



OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD
(8 CITINGS)

Accession Number

2002:198497 CAPLUS [Full-text](#)

Document Number

136:401857

Title

Acetylide-Bridged Organometallic Oligomers via the Photochemical Metathesis of Methyl-Iron(II) Complexes

Author/Inventor

Field, Leslie D.; Turnbull, Anthony J.; Turner, Peter

Patent Assignee/Corporate Source

School of Chemistry, The University of Sydney, Sydney, 2006, Australia

Source

Journal of the American Chemical Society (2002), 124(14), 3692-3702 CODEN: JACSAT; ISSN: 0002-7863

Document Type

Journal

Language

English

Abstract

The acetylide Me iron(II) complexes,

cis/trans-[Fe(dmpe)₂(C.tplbond.CR)(CH₃)] (1) and trans-[Fe(depe)₂(C.tplbond.CR)(CH₃)] (2) (dmpe = 1,2-dimethylphosphinoethane; depe = 1,2-diethylphosphinoethane), were synthesized by transmetalation from the corresponding alkyl halide complexes. Acetylide Me iron(II) complexes were also formed by transmetalation from the chloride complexes, trans-[Fe(dmpe)₂(C.tplbond.CR)(Cl)] or trans-[Fe(depe)₂(C.tplbond.CR)(Cl)]. The structure of trans-[Fe(dmpe)₂(C.tplbond.CC6H5)(CH₃)] (1a) was determined by single-crystal x-ray diffraction. The Me acetylide iron complexes, [Fe(dmpe)₂(C.tplbond.CR)(CH₃)] (1), are thermally stable in the presence of acetylenes, however, under UV irradiation, methane is lost with the formation of a metal bisacetylide. Photochem. metathesis of cis- or trans-[Fe(dmpe)₂(CH₃)(C.tplbond.CR)] [R = C₆H₅ (1a), 4-C₆H₄OCH₃ (1b)] with terminal acetylenes was used to selectively synthesize unsym. substituted iron(II) bisacetylide complexes of the type trans-[Fe(dmpe)₂(C.tplbond.CR)(C.tplbond.CR)] [R = Ph, R' = Ph (6a), 4-CH₃OC₆H₄ (6b), tBu (6c), SiMe₃ (6d), (CH₂)₄C.tplbond.CH (6e); R = 4-CH₃OC₆H₄, R' = 4-CH₃OC₆H₄, (6g), tBu (6h), (CH₂)₄C.tplbond.CH (6i), adamantyl (6j)]. The structure of the unsym. iron(II) bisacetylide complex trans-[Fe(dmpe)₂(C.tplbond.CC6H5)(C.tplbond.CC6H₄OCH₃)] (6b) was determined by single-crystal x-ray diffraction. The photochem. metathesis of the bis-acetylene, 1,7-octadiyne, with trans-[Fe(dmpe)₂(CH₃)(C.tplbond.CPh)] (1a), was utilized to synthesize the bridged binuclear species trans-trans-[(C₆H₅C.tplbond.C)Fe(dmpe)₂(μ-C.tplbond.C(CH₂)₄C.tplbond.C)Fe(dmpe)₂(C.tplbond.CC6H5)] (11). The trinuclear species trans,trans,trans-[(C₆H₅C.tplbond.C)Fe(dmpe)₂(μ-C.tplbond.C(CH₂)₄C.tplbond.C)Fe(dmpe)₂(μ-C.tplbond.C(CH₂)₄C.tplbond.C)Fe(dmpe)₂(C.tplbond.CC6H5)] (12) was synthesized by the photochem. reaction of Fe(dmpe)₂(C.tplbond.CPh)(C.tplbond.C(CH₂)₄C.tplbond.CH) (6e) with Fe(dmpe)₂(CH₃)₂. Extended irradiation of the bisacetylide complexes with phenylacetylene resulted in insertion of the terminal alkyne into one of the metal acetylide bonds to give acetylide butenyne complexes. The structure of the acetylide butenyne complex, trans-[Fe(dmpe)₂(C.tplbond.CC6H₄OCH₃)(η¹-C(C₆H₅)CH(C.tplbond.CC6H₄OCH₃))] (9a) was determined by single-crystal x-ray diffraction.

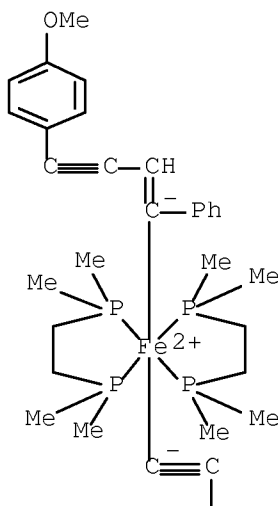
Hit Structure

CAS Registry Number
425390-70-7 CAPLUS

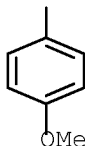
Chemical or Trade Name

Iron, bis[1,2-ethanediylbis(dimethylphosphine-κP)][(4-methoxyphenyl)ethynyl][(1E)-4-(4-methoxyphenyl)-1-phenyl-1-buten-3-ynyl]-, (OC-6-11)- (9CI) (CA INDEX NAME)

PAGE 1-A



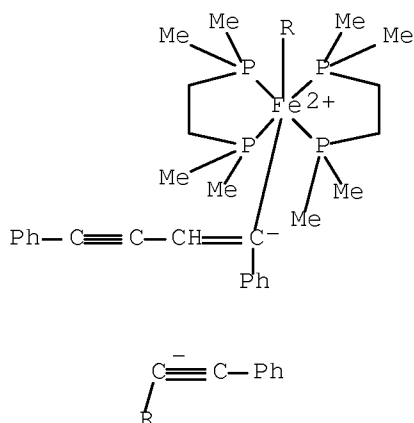
PAGE 2-A



CAS Registry Number
425390-85-4 CAPLUS

Chemical or Trade Name

Iron, [(1E)-1,4-diphenyl-1-buten-3-ynyl]bis[1,2-ethanediylbis(dimethylphosphine-κP)](phenylethynyl)-, (OC-6-11)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)

L4 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2001:714296 CAPLUS [Full-text](#)

Document Number

136.69640

Title

Synthesis and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units

Author/Inventor

Wan, W. Brad; Chiechi, Ryan C.; Weakley, Timothy J. R.; Haley, Michael M.

Patent Assignee/Corporate Source

Department of Chemistry and the Materials Science Institute, University of Oregon, Eugene, OR, 97403-1253, USA

Source

European Journal of Organic Chemistry (2001), (18), 3485-3490 CODEN: EJOCFK; ISSN: 1434-193X

Document Type

Journal

Language

English

Abstract

Dehydrobenzoannulene derivs. containing isolated alkene linkages, e.g., I, were synthesized by combining an in situ Pd/Cu-mediated cross-coupling with an intramol. cyclization strategy. ¹H NMR studies of these macrocycles and comparison with related systems verify that highly alkynylated dehydrobenzoannulenes possess weak induced ring currents, indicative of aromatic (4n+2 π systems) and antiarom. (4n π systems) behavior, in spite of their large size and extensive benzannulation.

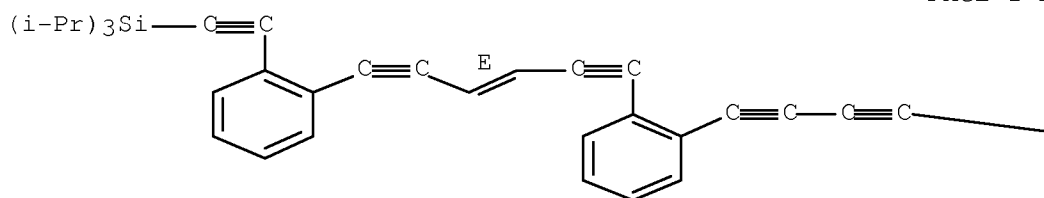
Hit Structure

CAS Registry Number

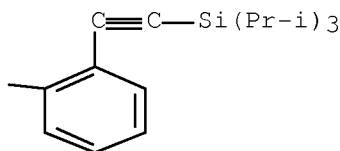
214628-17-8 CAPLUS

Chemical or Trade Name

Silane, tris(1-methylethyl)[[2-[(3E)-6-[2-[4-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-1,3-butadiynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)



PAGE 1-A



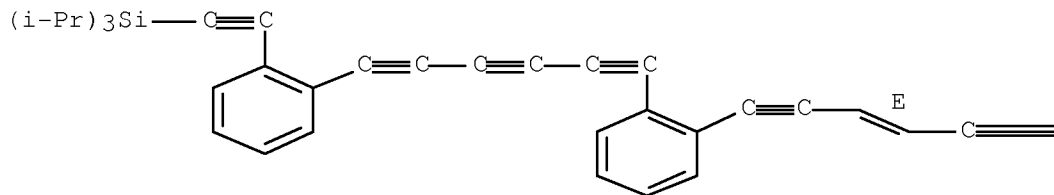
PAGE 1-B

CAS Registry Number

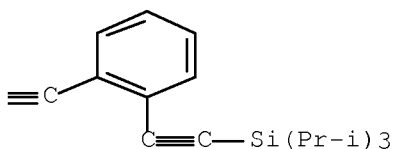
214628-18-9 CAPLUS

Chemical or Trade Name
 Silane, tris(1-methylethyl)[[2-[6-[2-[(3E)-6-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]-1,3,5-hexatriynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



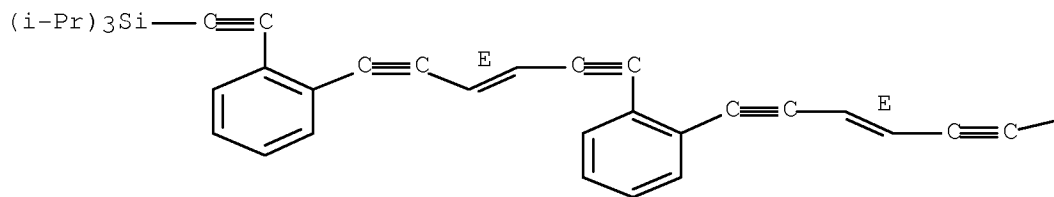
PAGE 1-B



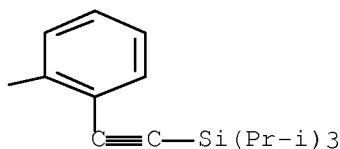
CAS Registry Number
 383404-38-4 CAPLUS

Chemical or Trade Name
 Silane, [1,2-phenylenebis[(3E)-3-hexene-1,5-diyne-6,1-diyl-2,1-phenylene-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L4 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number
 2000/832492 CAPLUS [Full-text](#)

Document Number
 134:310920

Title
 Bis(enediyne) Macrocycles: Synthesis, Reactivity, and Structural Analysis

Author/Inventor
 Blanchette, H. S.; Brand, S. C.; Naruse, H.; Weakley, T. J. R.; Haley, M. M.

Patent Assignee/Corporate Source
 Department of Chemistry, University of Oregon, Eugene, OR, 97403-1253, USA

Source
 Tetrahedron (2000), 56(49), 9581-9588 CODEN: TETRAB; ISSN: 0040-4020

Document Type
 Journal

Language

English

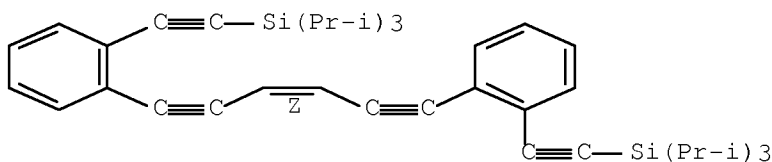
Abstract

The authors describe the syntheses of five macrocycles possessing two enediyne warheads, along with the structural and thermal analyses of these bis(enediyne) compds. The solid-state packing of one of the compds. suggests the possibility for the mol. to undergo a topochem. diacetylene polymerization

Hit Structure

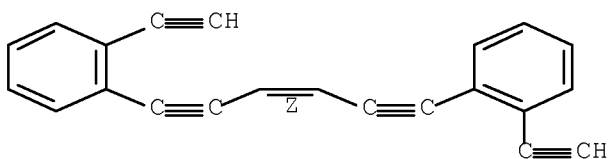
CAS Registry Number
335378-20-6 CAPLUS

Chemical or Trade Name
Silane, [(3Z)-3-hexene-1,5-diyne-1,6-diylbis(2,1-phenylene-2,1-ethynediyl)]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)



CAS Registry Number
335378-30-8 CAPLUS

Chemical or Trade Name
Benzene, 1,1'-(3Z)-3-hexene-1,5-diyne-1,6-diylbis[2-ethynyl- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)

.L4 .ANSWER 12 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2000:767122 CAPLUS [Full-text](#)

Document Number

134:71381

Title

Synthesis and structure of a new [6.6]metacyclophane with enediyne bridges

Author/Inventor

Srinivasan, Manivannan; Sankararaman, Sethuraman; Dix, Ina; Jones, Peter G.

Patent Assignee/Corporate Source

Department of Chemistry, Indian Institute of Technology, Madras, 600 036, India

Source

Organic Letters (2000), 2(24), 3849-3851 CODEN: ORLEF7; ISSN: 1523-7060

Document Type

Journal

Language

English

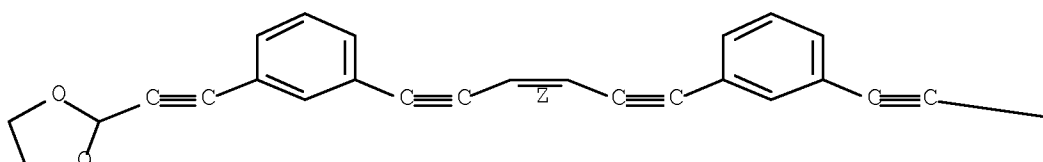
Abstract

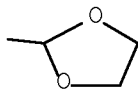
Synthesis and structure of a novel [6.6]metacyclophane with enediyne bridges I is reported. I was prepared by reacting 1,3-diethynylbenzene with EtMgBr/THF and DMF to give the monoaldehyde. The monoaldehyde was subsequently converted to the acetal, coupled with ClCH₂CHCl to give bis-acetal, which was hydrolyzed to the dialdehyde II. II underwent McMurry coupling using TiCl₃ and Zn-Cu couple in DME to give I in 69% yield.

Hit Structure

CAS Registry Number
315716-90-6 CAPLUS

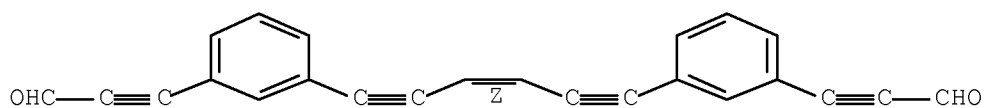
Chemical or Trade Name
1,3-Dioxolane, 2,2'-[(3Z)-3-hexene-1,5-diyne-1,6-diylbis(3,1-phenylene-2,1-ethynediyl)]bis- (9CI) (CA INDEX NAME)





CAS Registry Number
315716-91-7 CAPLUS

Chemical or Trade Name
2-Propynal, 3,3'-[(3Z)-3-hexene-1,5-diyne-1,6-diylid-3,1-phenylene]bis-
(9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 18 THERE ARE 18 CAPLUS RECORDS THAT CITE THIS
RECORD (18 CITINGS)

Accession Number

1999:673316 CAPLUS [Full-text](#)

Document Number

131:337589

Title

Electronic structure of fully conjugated dendritic oligomers of β,β -dibromo-4-ethynyl styrene

Author/Inventor

Fomine, Serguei; Fomina, Lioudmila; Guadarrama, Patricia

Patent Assignee/Corporate Source

Universidad Nacional Autonoma Mexico, Inst de Investigaciones en Materiales, Coyoacan, 04510 CU, Mex.

Source

Journal of Molecular Structure: THEOCHEM (1999), 488, 207-216 CODEN: THEODJ; ISSN: 0166-1280

Document Type

Journal

Language

English

Abstract

Quantum-mech. calcs. of fully conjugated dendritic oligomers carried out at B3LYP/3-21G/HF/3-21G (d) and B3LYP/3-21G/PM3 levels of theory showed that loose dendritic architecture of β,β -dibromo-4-ethynyl styrene oligomers contributes little to the instability and conjugation disruption compared to 1 \rightarrow 2 branched polyacetylene, while Br terminal atoms in dendrimers strongly affect the electronic d. distribution in studied mols. On the one hand the bulky bromine atoms decrease the conjugation in Br-terminated dendrimers caused by steric hindrances, on the other hand, highly polarizable bromine atoms reduced significantly adiabatic ionization potentials (IPa) to be up to 1.5 eV lower than corresponding vertical potentials (IPv). Another phenomenon contributing to the reducing of IPa's of all dendrimers is the flattening of mol. geometry accompanying the ionization thus allowing better delocalization of pos. charge over the conjugated system while all aromatic ring except the very outer layer lost their aromaticity becoming essentially quinone by nature.

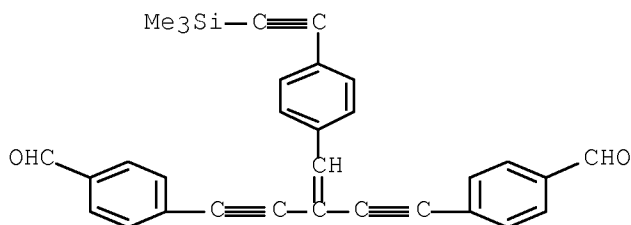
Hit Structure

CAS Registry Number

206181-71-7 CAPLUS

Chemical or Trade Name

Benzaldehyde, 4,4'-[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (9CI) (CA INDEX NAME)

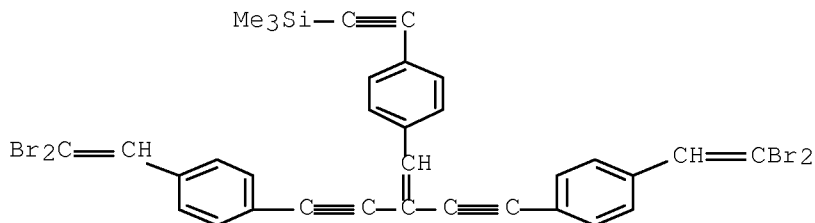


CAS Registry Number

206181-72-8 CAPLUS

Chemical or Trade Name

Silane, [[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)

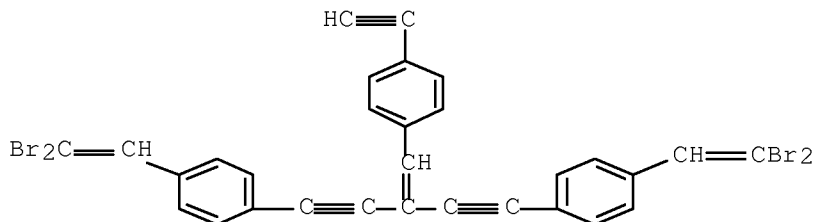


CAS Registry Number

206181-73-9 CAPLUS

Chemical or Trade Name

Benzene, 1,1'-[3-[[4-ethynylphenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4-(2,2-dibromoethenyl)- (9CI) (CA INDEX NAME)

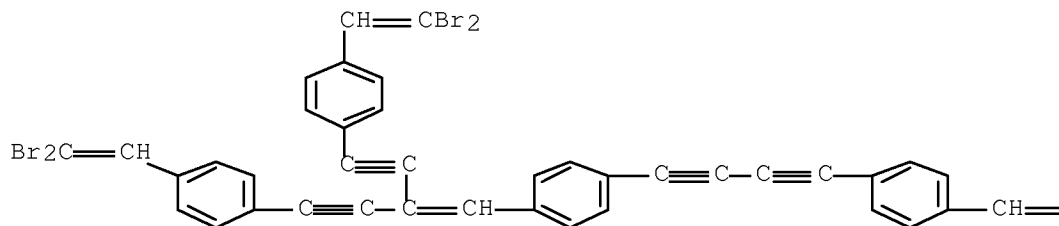


CAS Registry Number

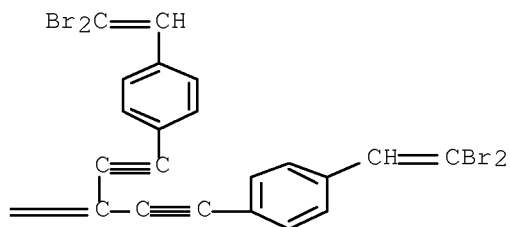
206181-74-0 CAPLUS

Chemical or Trade Name
Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

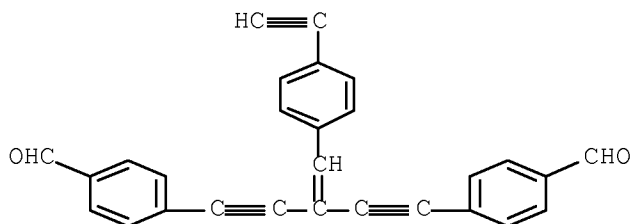


PAGE 1-B



CAS Registry Number
206181-75-1 CAPLUS

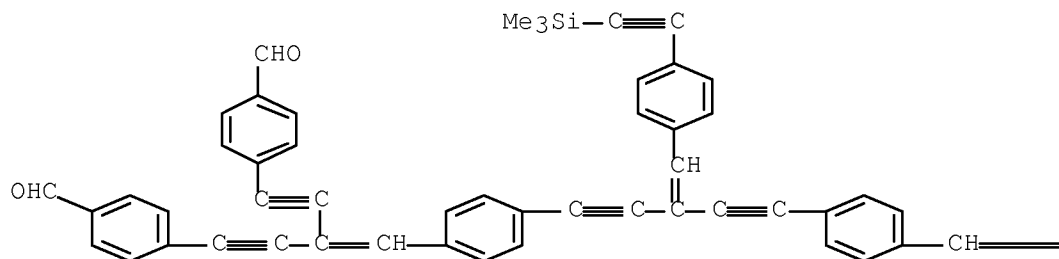
Chemical or Trade Name
Benzaldehyde, 4,4'-[3-[[4-ethynylphenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)

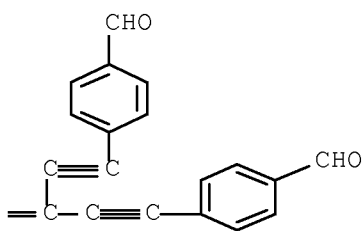


CAS Registry Number
206181-76-2 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[[4-formylphenyl]ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)

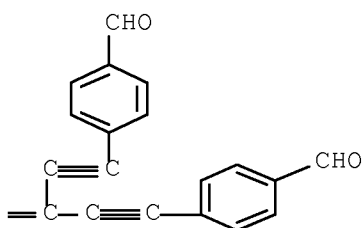
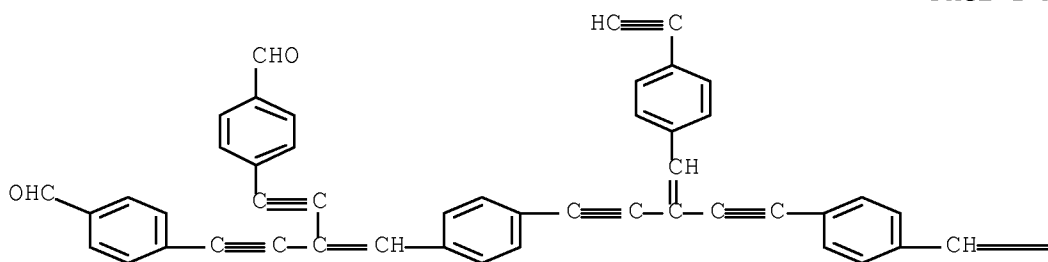
PAGE 1-A





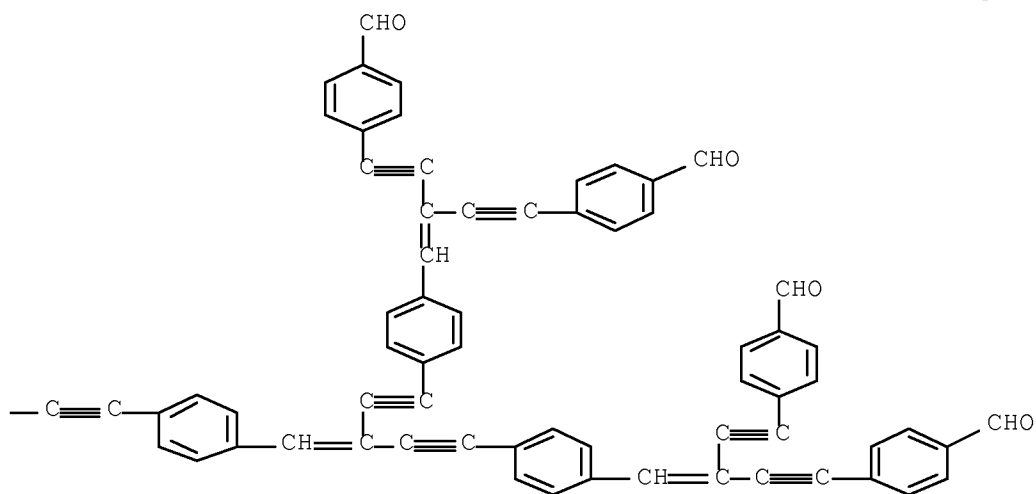
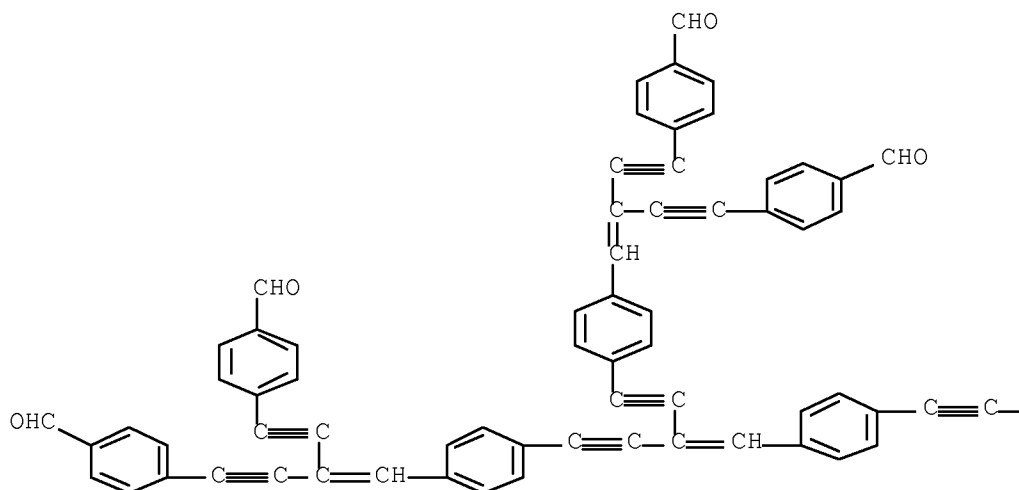
CAS Registry Number
206181-77-3 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[[3-[[4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



CAS Registry Number
206181-78-4 CAPLUS

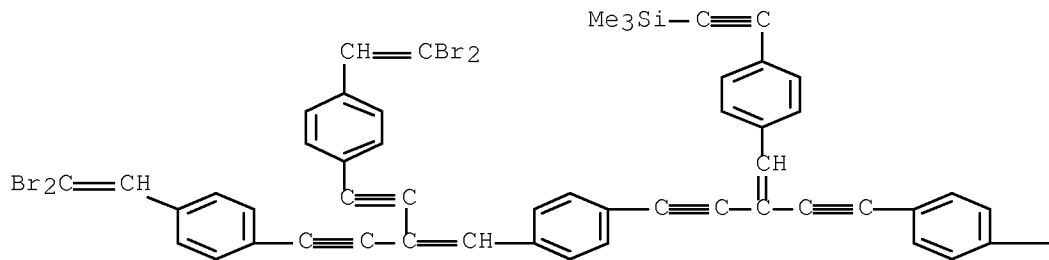
Chemical or Trade Name
Benzaldehyde, 4,4'-[[1,3-butadiyne-1,4-diyl]bis[4,1-phenylene[3-[[4-(4-formylphenyl)-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-3-buten-1-yne-4,1-diyl]-4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



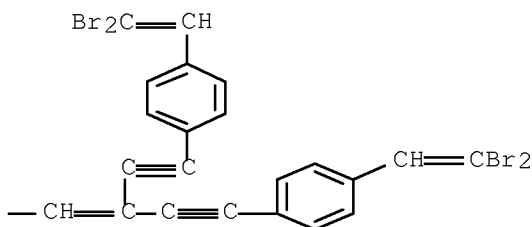
CAS Registry Number
206181-79-5 CAPLUS

Chemical or Trade Name
Silane, [[4-[[4-[[4-[[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD
(2 CITINGS)

L4 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1999:650836 CAPLUS [Full text](#)

Document Number

132:16702

Title

Theoretical description of luminescent effects in β,β -di(4'-formylphenylethynyl)-4-ethynylstyrene

Author/Inventor

Salcedo, R.; Guadarrama, P.; Sansores, L. E.; Fomine, S.; Fomina, L.

Patent Assignee/Corporate Source

Inst. de Investigaciones en Materiales, Inst. de Investigaciones en Materiales, UNAM, Mexico, 04510, Mex.

Source

Materials Research Society Symposium Proceedings (1999), 560(Luminescent Materials), 359-364 CODEN: MRSPDH; ISSN: 0272-9172

Document Type

Journal

Language

English

Abstract

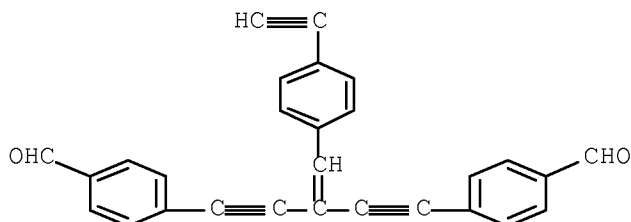
Theor. calcns. at HF/6-31 G(d) level were carried out on fully conjugated compds. (4-ethynylbenzaldehyde, β,β -dibromo-4-ethynylstyrene, β,β -Di(4'-formylphenylethynyl)-4-ethynylstyrene and its dimer) to understand the source of blue emission observed in oligomers of the 1st and 2nd generation in CHCl_3 solns. The frontier orbitals are distributed through the framework of the mols. (benzene rings, double and triple bonds and chromophores). Addnl., a CI approach was applied over β,β -Di(4'-formylphenylethynyl)-4-ethynylstyrene (compound 3) at CIS/6-31 G(d) level to modeling excited states and simulate the UV-visible spectrum exptl. obtained. Calculated transitions corresponded to $S_0 \rightarrow S_1$ which are, presumably, responsible for the fluorescence observed

Hit Structure

CAS Registry Number
206181-75-1 CAPLUS

Chemical or Trade Name

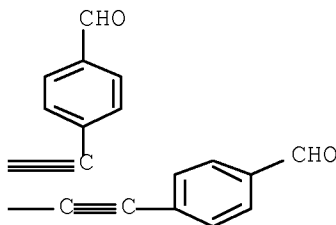
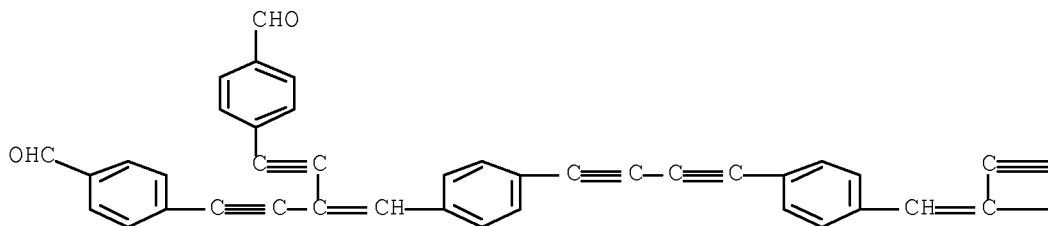
Benzaldehyde, 4,4'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



CAS Registry Number
251479-84-2 CAPLUS

Chemical or Trade Name

Benzaldehyde, 4,4'-[1,3-butadiyne-1,4-diylbis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L4 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1998:756297 CAPLUS [Full text](#)

Document Number

130:118607

Title

Porphyrin-[(E)-1,2-diethynylethene] scaffolding. Synthesis and optical and electrochemical properties of multinanometer-sized porphyrin arrays

Author/Inventor

Wyko, Jennifer; Berl, Volker; McLaughlin, Mark; Tykwinski, Rik R.; Schreiber, Martin; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice

Patent Assignee/Corporate Source

Laboratorium Organische Chemie, ETH-Zentrum, Zurich, CH-8092, Switz.

Source

Helvetica Chimica Acta (1998), 81(11), 1964-1977 CODEN: HCACAV; ISSN: 0018-019X

Document Type

Journal

Language

English

Abstract

Two series of linearly conjugated hybrid materials, consisting of (E)-1,2-diethynylethene (DEE; hex-3-ene-1,5-diyne) and Zn(II) porphyrin components, were prepared by Pd0-catalyzed cross-coupling reactions. In 1 series, 1 or 2 DEE substituents were introduced into the meso-positions of the Zn(II) porphyrins, leading from Zn 5,15-bis[(ethoxycarbonyl)propoxy]phenylporphinate (I) to I and II (n = 1; R = SiMe2tBu). The second series contains the linearly n-conjugated mol. rods III (n = 1-3) that span a length range from 23 Å for III (n = 1) to 53 Å for III (n = 3). The larger rods III (n = 2 and 3) consist of 2 or 3 porphyrin moieties, resp., that are bridged at the meso-positions by trans-enediynediyl (hex-3-ene-1,5-diyne-1,6-diyl) linkers. The UV/VIS spectra in the series I, II, and III (n = 1) showed a strong bathochromic shift of both Soret and Q bands of the Zn(II) porphyrin as a result of the addition of DEE substituents. Upon changing from I to II, the Q band was further bathochromically shifted, whereas the Soret band remained nearly at the same position but became broadened and displayed a shoulder on the lower-wavelength edge as a result of excitonic coupling. The close resemblance between the UV/Vis spectra of III (n = 2 and 3) suggests that saturation of the optical properties in the oligomeric series already occurs at the stage of dimeric III (n = 2). Stationary voltammetric investigations showed that the DEE substituents act as strong electron acceptors which induce large anodic shifts in the 1st reduction potential upon changing from I to II ($\Delta E = 190$ mV) and to III (n = 1) ($\Delta E = 340$ mV). Increasing the number of porphyrin moieties upon changing from III (n = 1) to III (n = 2) had no effect on the 1st reduction potential yet the 1st oxidation potential was substantially lowered ($\Delta E = 110$ mV). Large differences in the potentials for 1-electron oxidation of the 2 porphyrin moieties in III (n = 2) ($\Delta E = 200$ mV) confirmed the existence of substantial electronic communication between the 2 macrocycles across the trans-enediynediyl bridge.

Hit Structure

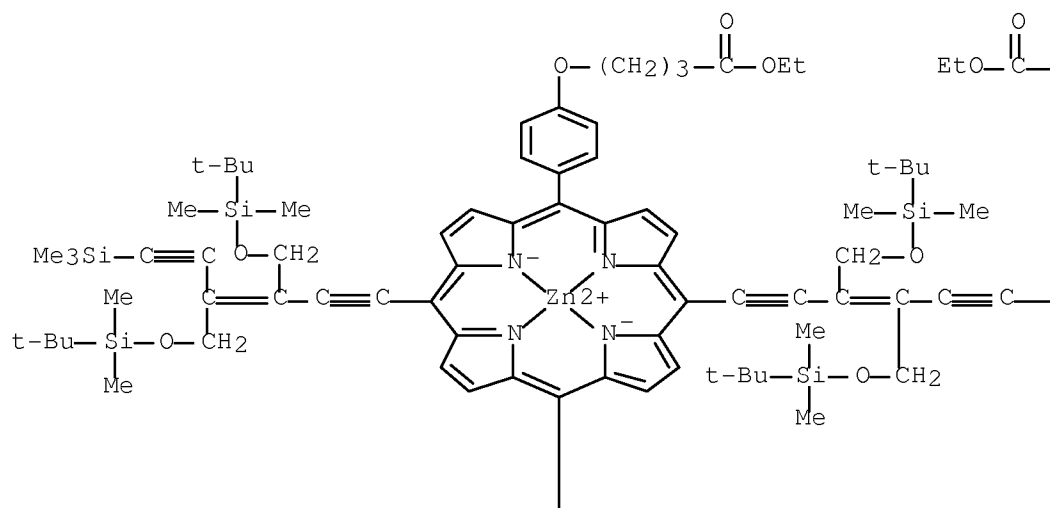
CAS Registry Number

219483-19-9 CAPLUS

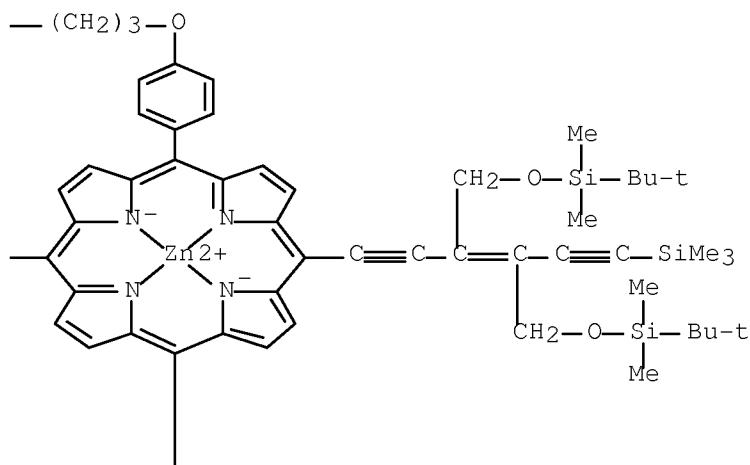
Chemical or Trade Name

Zinc, [μ -[[[tetraethyl 4,4',4'',4'''-[[[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyne-1,6-diyl]bis[[20-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyne]-21H,23H-porphine-10,5,15-triyl- κ N21, κ N22, κ N23, κ N24]-4,1-phenyleneoxy]]tetrakis[butanoato]](4-)]]]di- (9CI) (CA INDEX NAME)]

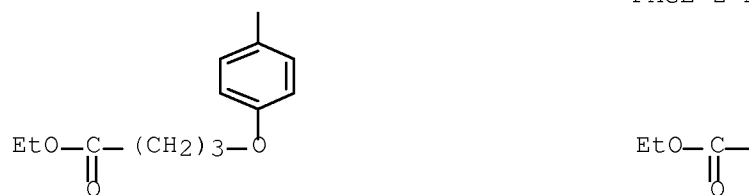
PAGE 1-A

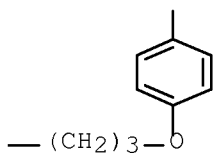


PAGE 1-B



PAGE 2-A





OS.CITTING REF COUNT: 45 THERE ARE 45 CAPLUS RECORDS THAT CITE THIS RECORD (45 CITINGS)

L4 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1998:606810 CAPLUS [Full-text](#)

Document Number

129:302407

Title

Synthesis of expanded planar dehydrobenzoannulenes: weakly diatropic, weakly paratropic, or atropic?

Author/Inventor

Wan, W. Brad; Kimball, David B.; Haley, Michael M.

Patent Assignee/Corporate Source

Department of Chemistry, University of Oregon, Oregon, 97403-1253, USA

Source

Tetrahedron Letters (1998), 39(38), 6795-6798 CODEN: TELEAY; ISSN: 0040-4039

Document Type

Journal

Language

English

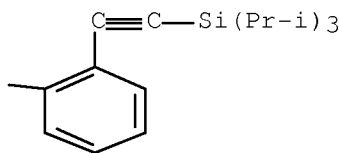
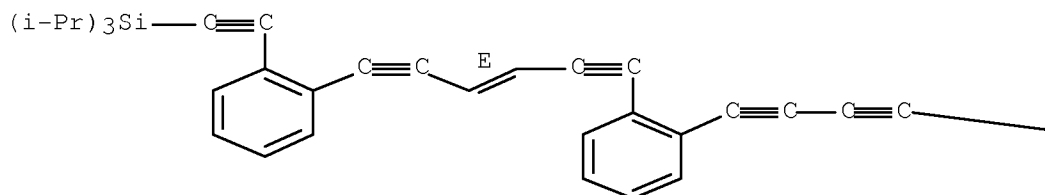
Abstract

Use of a Cu/Pd cross-coupling strategy has led to the synthesis of the first dehydrobenzoannulenes [X = C, (E)-CH=CH; n = 0, 1] containing triacetylenic linkages. NMR studies of these macrocycles and comparison with other known systems indicate that, in spite of their large size and extensive benzannellation, dehydrobenzoannulenes possess weak induced ring currents.

Hit Structure

CAS Registry Number
214628-17-8 CAPLUS

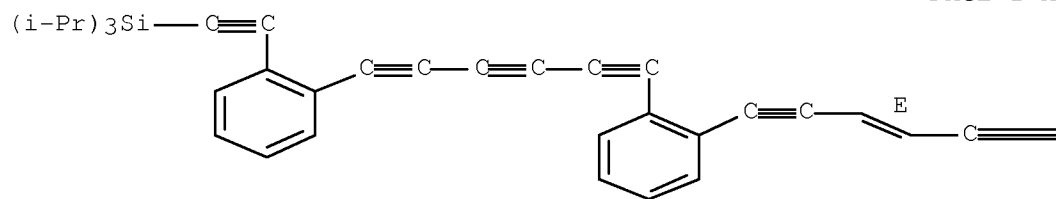
Chemical or Trade Name
Silane, tris(1-methylethyl)[{2-[(3E)-6-[2-[4-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-butadiynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)



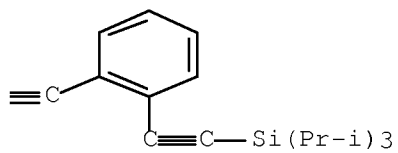
CAS Registry Number
214628-18-9 CAPLUS

Chemical or Trade Name
Silane, tris(1-methylethyl)[{2-[6-[2-[(3E)-6-[2-[[tris(1-methylethyl)silyl]ethynyl]phenyl]-3-hexene-1,5-diynyl]phenyl]-1,3,5-hexatriynyl]phenyl]ethynyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 26 THERE ARE 26 CAPLUS RECORDS THAT CITE THIS
RECORD (27 CITINGS)

L4 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1998:269262 CAPLUS [Full-text](#)

Document Number

128:257221

Title

Steric Hindrance Facilitated Synthesis of Enynes and Their Intramolecular [4 + 2] Cycloaddition with Alkynes

Author/Inventor

Gonzalez, Juan J.; Francesch, Andres; Cardenas, Diego J.; Echavarren, Antonio M.

Patent Assignee/Corporate Source

Departamento de Química Organica, Universidad Autonoma de Madrid, Madrid, 28049, Spain

Source

Journal of Organic Chemistry (1998), 63(9), 2854-2857 CODEN: JOCEAH; ISSN: 0022-3263

Document Type

Journal

Language

English

Abstract

The palladium-catalyzed insertion of 1-alkynes into internal alkynes which are bent out of linearity by the interference with a peri or ortho substituent led to enynes regioselectively. The resulting enynes undergo a new type of intramol. thermal cycloaddn., which can be used for the annulation of an aryl ring onto naphthalene derivs. to afford fluranthenes. The cyclization of (E)-1-(1-buten-3-ynyl)-8-ethynynaphthalene could also be performed in the presence of a Cu(I) catalyst at room temperature

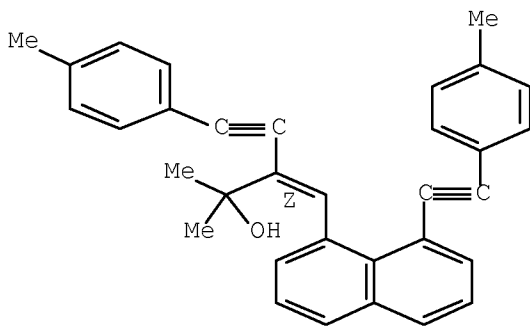
Hit Structure

CAS Registry Number

205124-39-6 CAPLUS

Chemical or Trade Name

4-Pentyn-2-ol, 2-methyl-5-(4-methylphenyl)-3-[[8-[2-(4-methylphenyl)ethynyl]-1-naphthalenyl]methylene]-, (3Z)- (CA INDEX NAME)



OS.CITING REF COUNT: 23 THERE ARE 23 CAPLUS RECORDS THAT CITE THIS RECORD (23 CITINGS)

L4 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1998:247633 CAPLUS [Full-text](#)

Document Number

128:295129

Title

Synthesis and characterization of well-defined fully conjugated hyperbranched oligomers of β,β -dibromo-4-ethynylstyrene

Author/Inventor

Fomina, Lioudmila; Guadarrama, Patricia; Fomine, Serguei; Salcedo, Roberto; Ogawa, Takeshi

Patent Assignee/Corporate Source

Instituto Investigaciones Materiales, Univ. Nacional Autonoma de Mexico, Mexico, 04510, Mex.

Source

Polymer (1998), 39(12), 2629-2635 CODEN: POLMAG; ISSN: 0032-3861

Document Type

Journal

Language

English

Abstract

Well-defined dendritic oligomers of poly(β,β -dibromo-4-ethynylstyrene) of the first and second generation were synthesized by a stepwise synthesis, and characterized. NMR and theor. calcons. showed that free rotation around formal single bonds is hampered by conjugation. All of the oligomers were blue emitters with their emission maxima correlating with the number of repeating units. All dendrimers except β,β -bis[β',β' -di(β'' - β'' -dibromostyryl)-4'-ethynyl]styryl-4'-ethynyl]-4-ethynylstyrene showed two maxima in the excitation spectra.

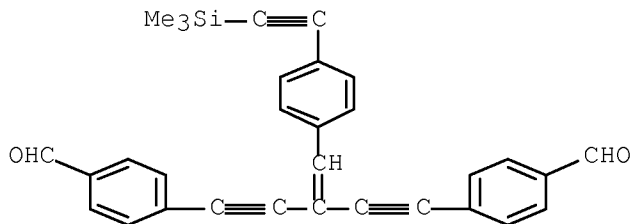
Hit Structure

CAS Registry Number

206181-71-7 CAPLUS

Chemical or Trade Name

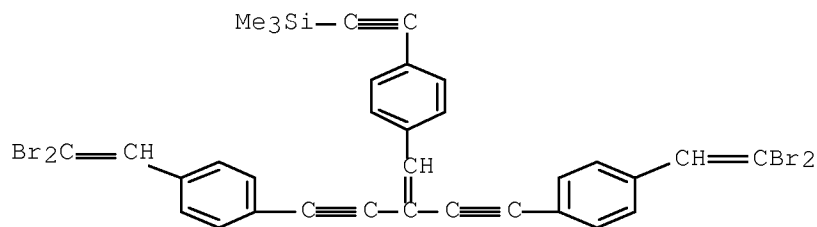
Benzaldehyde, 4,4'-[3-[[4-[(trimethylsilyl)ethynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (9CI) (CA INDEX NAME)



CAS Registry Number
206181-72-8 CAPLUS

Chemical or Trade Name
Silane, [[4-[4-[4-(2,2-dibromoethenyl)phenyl]phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl-

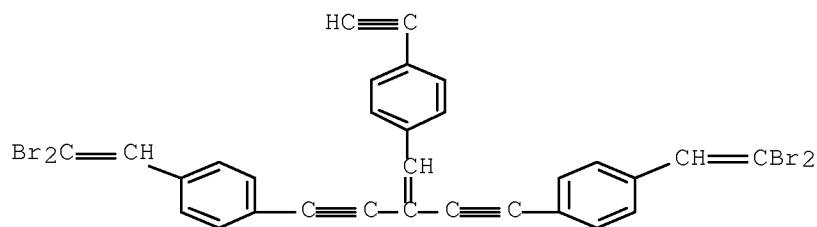
(9CI) (CA INDEX NAME)



CAS Registry Number
206181-73-9 CAPLUS

Chemical or Trade Name
Benzene, 1,1'-[3-[[4-(ethynyl)phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4-(2,2-dibromoethenyl)-

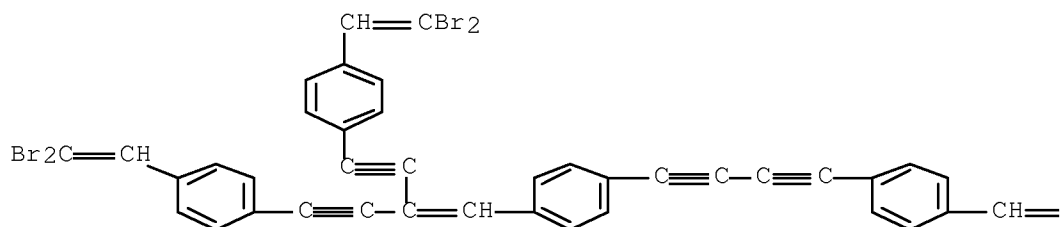
(9CI) (CA INDEX NAME)



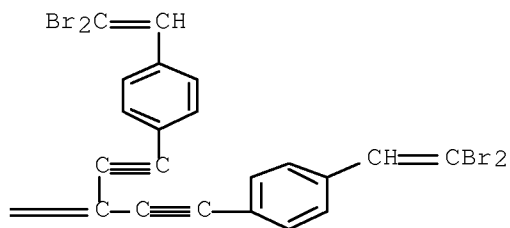
CAS Registry Number
206181-74-0 CAPLUS

Chemical or Trade Name
Benzene, 1,1'-[(1,3-butadiyne-1,4-diyl]bis[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]-

(9CI) (CA INDEX NAME)



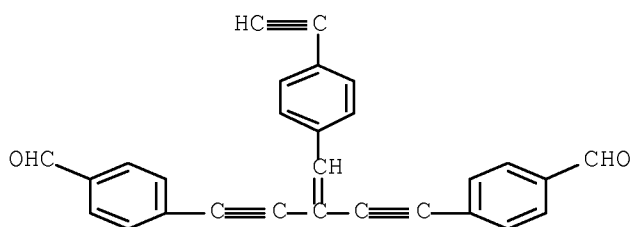
PAGE 1-A



PAGE 1-B

CAS Registry Number
206181-75-1 CAPLUS

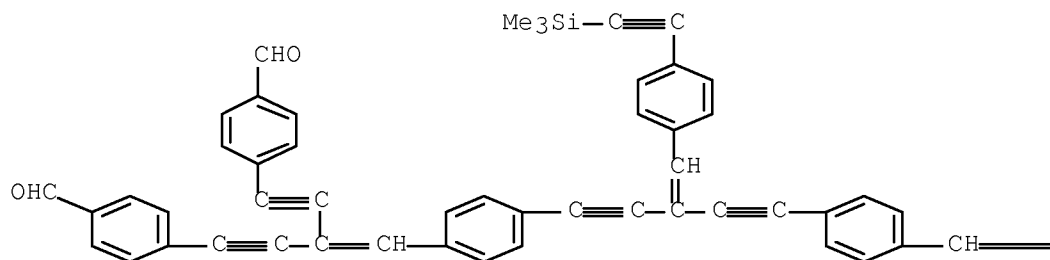
Chemical or Trade Name
Benzaldehyde, 4,4'-[3-[(4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis- (CA INDEX NAME)



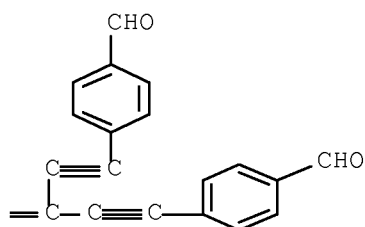
CAS Registry Number
206181-76-2 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[[3-[[4-[(trimethylsilyl)ethynyl]phenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)

PAGE 1-A



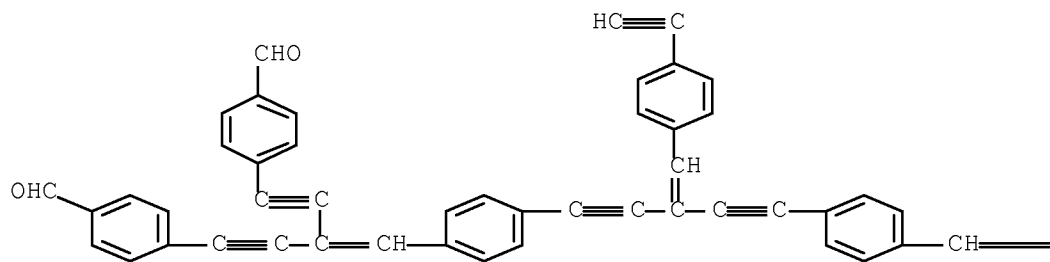
PAGE 1-B



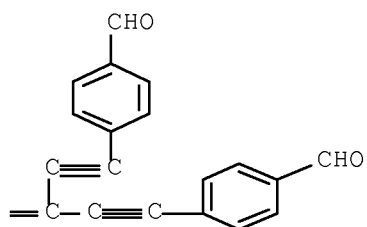
CAS Registry Number
206181-77-3 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[[3-[[4-ethynylphenyl)methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]]bis- (9CI) (CA INDEX NAME)

PAGE 1-A



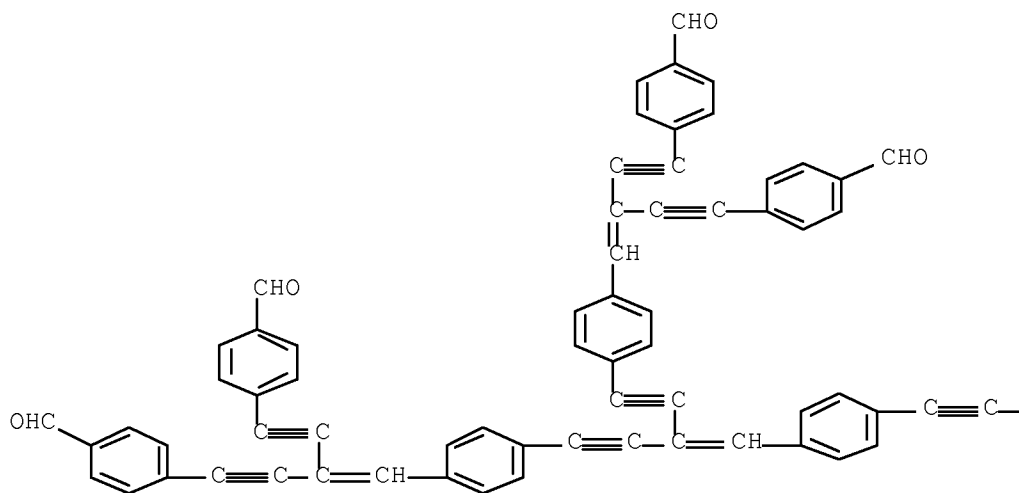
PAGE 1-B

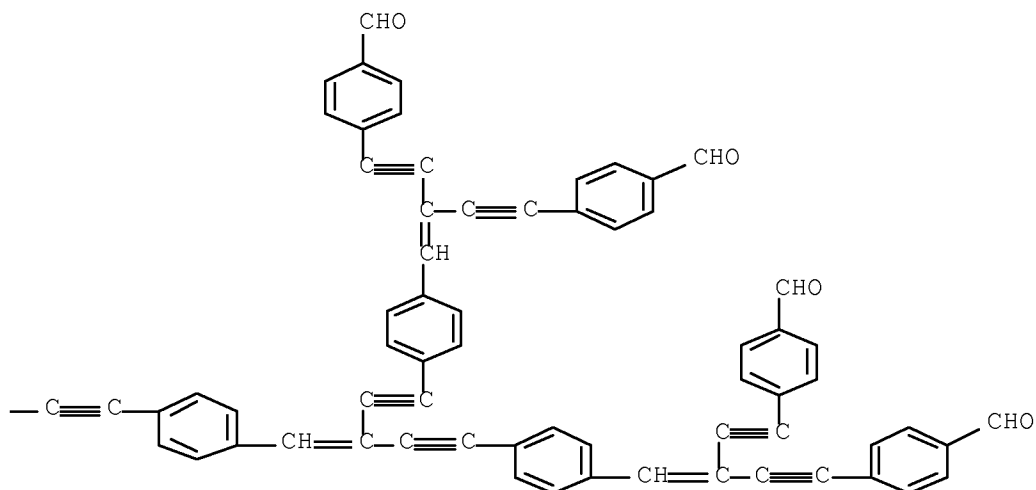


CAS Registry Number
206181-78-4 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[1,3-butadiyne-1,4-diylbis[4,1-phenylene[3-[[4-[4-(4-formylphenyl)-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-3-buten-1-yne-4,1-diyl]-4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

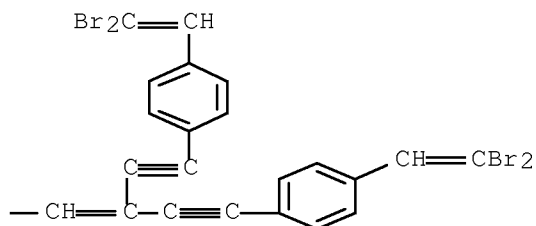
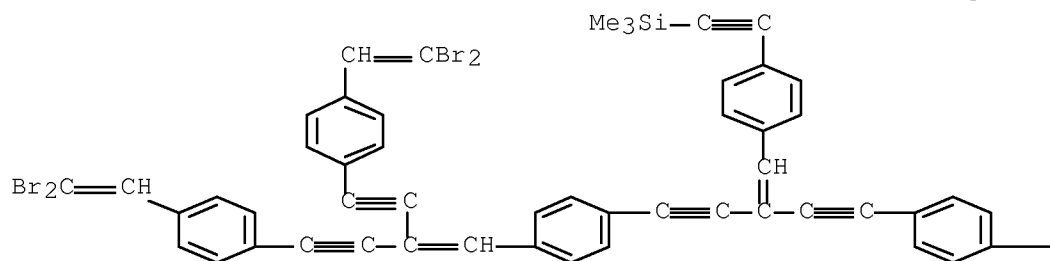
PAGE 1-A





CAS Registry Number
206181-79-5 CAPLUS

Chemical or Trade Name
Silane, [[4-[[4-[[4-[[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-[[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]trimethyl- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L4 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number
1996-303100 CAPLUS E41:381

Document Number
125:11582

Title
Synthesis and polymerization of β,β -dibromo-4-ethynylstyrene; preparation of a new polyconjugated, hyperbranched polymer
Author/Inventor
Fomina, Lioudmila; Salcedo, Roberto

Patent Assignee/Corporate Source
Inst. Investigaciones Materiales, Circuito Exterior, Ciudad Univ., Mexico City, 04510, Mex.

Source
Polymer (1996), 37(9), 1723-1728 CODEN: POLMAG; ISSN: 0032-3861

Document Type
Journal

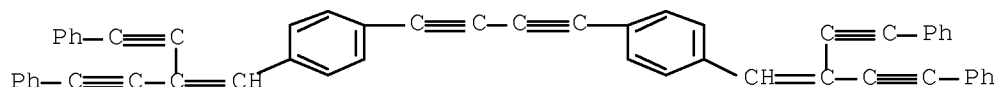
Language
English

Abstract
The monomer, β,β -dibromo-4-ethynylstyrene, was prepared and polymerized by the Heck reaction to give a partially soluble, conjugated hyperbranched polymer. The polymer structure was elucidated using standard spectroscopic techniques and with the aid of model compound synthesis. Theor. calcs. using the AM1 method were carried out and showed that conjugation in the polymer is partially disrupted by twisting of the benzene rings. Both the model compound and the polymer showed luminescence.

Hit Structure

CAS Registry Number
177410-40-1 CAPLUS

Chemical or Trade Name
Benzene, 1,1'-(1,3-butadiyne-1,4-diyl)bis[4-[4-phenyl-2-(phenylethynyl)-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)



OS.CITING REF COUNI: 16 THERE ARE 16 CAPLUS RECORDS THAT CITE THIS RECORD (16 CITINGS)

L4 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number
1995:945580 CAPLUS [Full Text](#)

Document Number
124:9540

Title
Novel polymers containing discrete conjugated units, produced by the Heck reaction

Author/Inventor
Fomine, Sergei; Fomina, Lioudmila; Florentino, Hector Quiroz; Mendez, Juan Manuel; Ogawa, Takeshi

Patent Assignee/Corporate Source
Instituto de Investigaciones en Materiales, Universidad Nacional Autonoma de Mexico, Coyoacan, 04510, Mex.

Source
Polymer Journal (Tokyo) (1996), 27(11), 1085-93 CODEN: POLJB8; ISSN: 0032-3896

Document Type
Journal

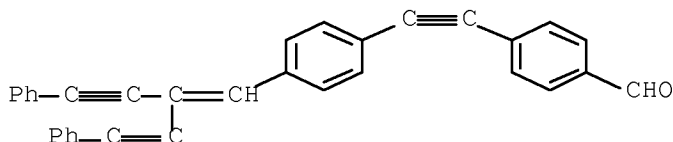
Language
English

Abstract
Novel monomers and polymers containing arylenevinylideneethynylene groups were synthesized via the Heck reaction. The polymers were amorphous and soluble in common organic solvents. They have Tg approx. 60°, 5% weight loss at 240-340° and undergo thermal crosslinking at 170-190° with loss of triple bonds. One of the polymers exhibits strong blue luminescence with emission maxima approx. 380-390 and 470-480 nm with excitation at 320 nm. All polymers show 3rd order NLO susceptibility approx. 10-10 esu.

Hit Structure

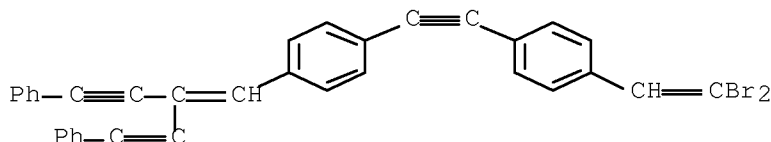
CAS Registry Number
171296-95-0 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4-[2-[4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]phenyl]ethynyl]- (CA INDEX NAME)



CAS Registry Number
171296-96-1 CAPLUS

Chemical or Trade Name
Benzene, 1-[2-[4-(2,2-dibromoethenyl)phenyl]ethynyl]-4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



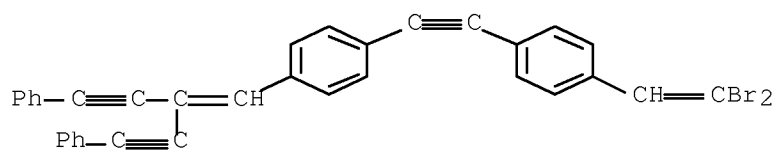
CAS Registry Number
171296-99-4 CAPLUS

Chemical or Trade Name
Decanedioic acid, di-2-propynyl ester, polymer with 1-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-4-[4-phenyl-2-(phenylethynyl)-1-

buten-3-ynyl]benzene (9CI) (CA INDEX NAME)

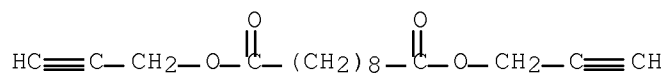
CM
1

CRN 171296-96-1
CMF C34 H20 Br2



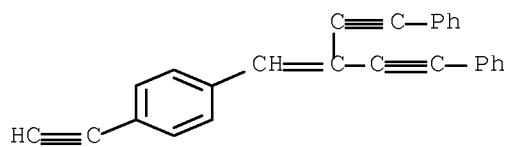
CM
2

CRN 93164-22-8
CMF C16 H22 O4



CAS Registry Number
171297-02-2 CAPLUS

Chemical or Trade Name
Benzene, 1-ethynyl-4-[[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]]-
(CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS
RECORD (11 CITINGS)

L4 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1995:642218 CAPLUS [Full-text](#)

Document Number

123:33763

Title

Synthesis and molten-state polymerization of some novel conjugated diacetylenes

Author/Inventor

Fomina, Lioudmila; Allier, Hector; Fomine, Sergei; Salcedo, Roberto; Ogawa, Takeshi

Patent Assignee/Corporate Source

Inst. Investigaciones Materiales, Ciudad Univ., Mexico, 04510, Mex.

Source

Polymer Journal (Tokyo) (1995), 27(6), 591-600 CODEN: POLJ88; ISSN: 0032-3896

Document Type

Journal

Language

English

Abstract

A series of new, highly conjugated diacetylenes, 4-ethynylstilbene derivs., was synthesized and their polymerization was studied. None of them was found to undergo topochem. polymerization in the solid state but they readily polymerized in the molten state to give red transparent and amorphous polymers. All the polymers had an absorption maximum in the visible spectra around 500 nm, and FT-IR data showed the enyne structure of the polymer chain resulted from 1,4-addition

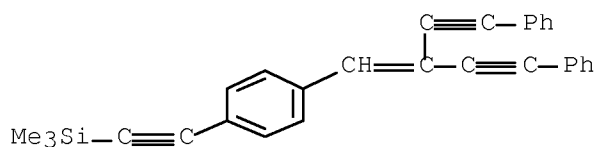
Hit Structure

CAS Registry Number

164467-30-5 CAPLUS

Chemical or Trade Name

Benzene, 1-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]-4-[2-(trimethylsilyl)ethynyl]- (CA INDEX NAME)



CAS Registry Number

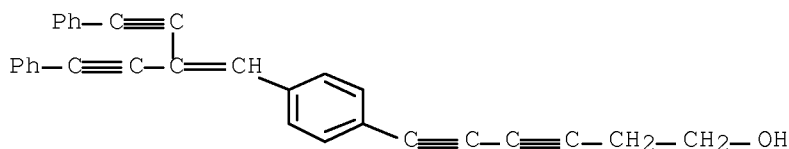
164467-25-8 CAPLUS

Chemical or Trade Name

3,5-Hexadiyn-1-ol, 6-[4-[4-phenyl-2-(phenylethynyl)-1-buten-3-ynyl]phenyl]-, homopolymer (9CI) (CA INDEX NAME)

CM
1

CRN 164467-20-3
CMF C30 H20 O

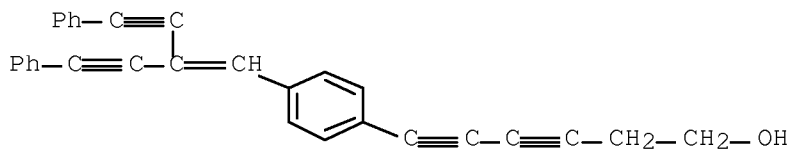


CAS Registry Number

164467-20-3 CAPLUS

Chemical or Trade Name

3,5-Hexadiyn-1-ol, 6-[4-[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]phenyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

L4 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1994:522234 CAPLUS [Full-text](#)

Document Number

121:122234

Title

Diffuoride derivative and liquid crystal composition containing the same

Author/Inventor

Yokokoji, Osamu; Irisawa, Jun; Koh, Hidemasa

Patent Assignee/Corporate Source

Asahi Glass Co., Ltd., Japan
Source
PCT Int. Appl., 43 pp. CODEN: PIXXD2
Document Type
Patent
Language
Japanese
Patent Information

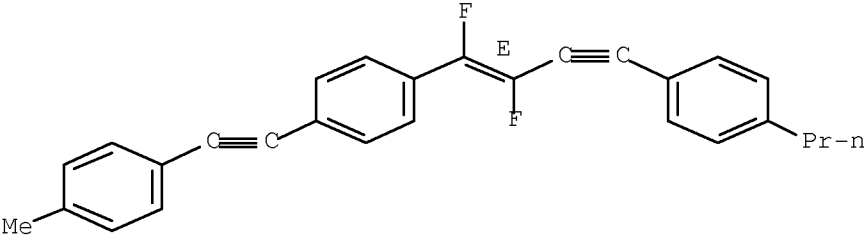
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9405613	A1	19940317	WO 1993-JP1235	19930901
EP 628528	A1	19941214	EP 1993-919602	19930901
JP 06263661	A	19940920	JP 1993-219709	19930903
JP 3564711	B2	20040915		
US 5419851	A	19950530	US 1994-211625	19940420
JP 2004292454	A	20041021	JP 2004-115211	20040409
JP 3707493	B2	20051019		

Abstract
Difluoride derivs. represented by the general formula: R1(A1Y1)mA2CF:CFC.tplbond.CA3(Y2A4)nR2 (A1 - A4 = trans-1,4-cyclohexylene, 1,4-cyclohexenylene, or 1,4-phenylene wherein ≥1 CH groups of each ring may be substituted by N or ≥1 CH2 groups of the ring may be substituted by O or S; m, n = 0, 1; R1, R2 = C1-10 alkyl, halo, cyano wherein (1) O, CO2, or O2C may be inserted between the C-C bond of alkyl or that between alkyl and ring, (2) a part of the C-C bonds in alkyl is replaced by C:C or C.tplbond.C bond, or (3) one CH2 group in alkyl is replaced by CO group; Y1, Y2 = CO2, O2C, C.tplbond.C, CH2CH2, CHCH, OCH2, CH2O) are prepared. These compds. have low viscosity, are light-stable, and hence can provide a liquid crystal composition having high response speed. Thus, 0.1 mol ClCF:CF2 was blown into THF at -100° followed by adding dropwise 62.1 mL 1.61 M BuLi/hexane, stirring for 30 min, adding dropwise 0.1 mol Me3SiCl, stirring for 1 h, adding dropwise a solution of 4-propylphenyl lithium in THF (prepared from 4-propyliodobenzene and BuLi) at -100°, and stirring for 2 h at 0° to give 75% (Z)-4-PrC6H4CF:CFSiMe3. The latter compound (0.075 mol) was reacted with 0.15 mol KF in aqueous MeCN at 70° for 1 h to give 83% (E)-4-PrC6H4CF:CFH which (0.062 mol) was dissolved in THF, cooled to -78°, and treated dropwise with 38.5 mL 1.61 M BuLi/hexane followed by stirring for 30 min, adding 15.7 g iodine, and stirring at room temperature for 4 h to give 83% (E)-4-PrC6H4CF:CFI. The latter compound (0.051 mol) and 0.051 mol 4-propylphenylacetylene were dissolved in 100 mL Et3N followed by adding Pd(PPh3)2Cl2 and CuI and the resulting mixture was allowed to react at room temperature for 6 h to give 70% diphenyldifluorobutenyne derivative (I). A STN-type liquid crystal display device was prepared from a liquid composition containing 20 weight% I and 80 weight% ZLI-1565 and irradiated with a UV carbon arc lamp for 200 h; new compds. were hardly formed whereas cis-4,4'-bis(n-propyl)difluorostilbene was formed in a liquid crystal composition containing ZLI-1565 and trans-4,4'-bis(n-propyl)difluorostilbene.

Hit Structure

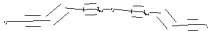
CAS Registry Number
156869-08-8 CAPLUS

Chemical or Trade Name
Benzene, 1-[1,2-difluoro-4-(4-propylphenyl)-1-buten-3-ynyl]-4-[(4-methylphenyl)ethynyl]-, (E)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(5 CITINGS)

=>

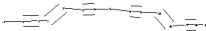


chain nodes :
1 2 3 4 5 6 7 8 9 11 15 16 17 18 19
chain bonds :
1-2 1-11 2-3 3-4 4-5 5-6 6-7 7-8 8-9 9-15 15-16 16-17 17-18 18-19
exact/norm bonds :
1-11 6-7 7-8 18-19
exact bonds :
1-2 2-3 3-4 4-5 5-6 8-9 9-15 15-16 16-17 17-18

G1:Cb,Cy,Hy

G2:C,H,Si,Cb,Cy,Hy

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 8:CLASS 9:CLASS 11:Atom 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom



L5 STRUCTURE UPLOADED
=> s 15 sss full
FULL SEARCH INITIATED 12:52:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 12029 TO ITERATE
100.0% PROCESSED 12029 ITERATIONS 72 ANSWERS
SEARCH TIME: 00.00.01

L6 72 SEA SSS FUL L5

=> s 16

L7 23 L6

=> 17 and (py<=2004 or ay<=2004)

25158915 FY<=2004

5170681 AY<=2004

L8 14 L7 AND (FY<=2004 OR AY<=2004)

=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 14 ANSWERS - CONTINUE? Y/(N):y

L8 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

200534387 CAPLUS [Full-text](#)

Document Number

142:135171

Title

Liquid crystalline compound having perfluoroalkyl side chains, liquid crystal composition containing these compounds and their polymers

Author/Inventor

Sasada, Yasuyuki; Yanai, Motoki

Patent Assignee/Corporate Source

Chisso Petrochemical Corporation, Japan; Chisso Corporation

Source

U.S. Pat. Appl. Publ., 56 pp. CODEN: USXXCO

Document Type

Patent

Language

English

Patent Information

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050007541	A1	20050113	US 2004-873280	20040623
US 7070838	B2	20060704		
JP 2005035985	A	20050210	JP 2004-183449	20040622

Abstract

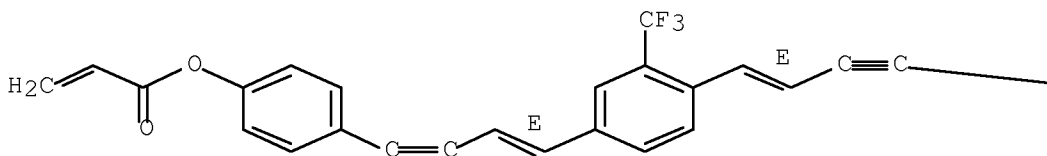
Liquid crystalline compds. I [P = CX22: CX1CO2, Q1, CX22: CX2O, p-CX22: CX2COC6H4, or Q2; A1 = 1,4-cyclohexenylen, 1,4-phenylene, naphthalene-2,6-diyl, tetrahydronaphthalene-2,6-diyl, fluorene-2,7-diyl, or bicyclo[2.2.2]octane-1,4-diyl, where any CH2 of these rings is optionally replaced by O, any CH is optionally replaced by N,; and any H is optionally replaced by halo, C1-5 alkyl, or halogenated alkyl; Z1 = single bond, CH2CH2, CF2CF2, (CH2)4, CH2O, OCH2, CO2, OCO, CH:CH, CF:CF, C:iplbond.C, C:iplbond.CCO2, COOC:iplbond.C, CH:CHCO2, COOCH:CH, CH2CH2CO2, COOCH2CH2, C:iplbond.CCH:CH, CH:CHC:iplbond.C, OCF2, or CF2; Z2 = single bond or C1-20 alkylene, where any CH2 is optionally replaced by O, S, CO2, or OCO; X1 = H, halo, CF3 or C1-5 alkyl, X2 = H, halo, or C1-5 alkyl; m, n = 0-2; m + n ≤ 4; p = 2 or 3; q = 0 or 1; when Z1 is C:iplbond.C, P = Q1, CX22: CX2O, p-CX22: CX2COC6H4] are prepared. The invention further provides for polymerization of a composition containing z1 of I to give a film, an optical anisotropic material, a 1/4 or 1/2 wavelength functional plate, an optical compensation element, an optical element or a liquid crystal display element. A typical liquid crystalline compound (I) was manufactured by esterification of 2-(trifluoromethyl)-1,4-dihydroxybenzene with 4-[6-(acryloyloxy/hexyloxy)benzoic acid in THF in the presence of 4-dimethylaminopyridine and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide overnight. A typical liquid crystalline polymer was manufactured by photopolymer. of 80 parts II in a mixture containing 4-(trans-4-propylcyclohexyl)cyanobenzene 5, 4-(trans-4-pentylcyclohexyl)cyanobenzene 5, 4-(trans-4-heptylcyclohexyl)cyanobenzene 5, and 4'-(trans-4-heptylcyclohexyl)-4-cyano-1,1'-biphenyl 5 parts in the presence of ligacure 907 as a film on a polyimide alignment film attached to a glass substrate.

Hit Structure

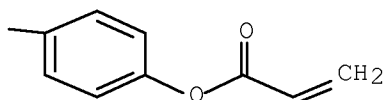
CAS Registry Number
1056056-84-8 CAPLUS

Chemical or Trade Name
INDEX NAME NOT YET ASSIGNED

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L8 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2004566840 CAPLUS [Full-text](#)

Document Number

141:261152

Title

π -Conjugated Dendrimers Based on Bis(enediynyl)benzene Units

Author/Inventor

Hwang, Gil Tae; Kim, Byeang Hyeon

Patent Assignee/Corporate Source

National Research Laboratory, Department of Chemistry, Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

Source

Organic Letters (2004), 6(16), 2669-2672 CODEN: ORLEF7; ISSN: 1523-7060

Document Type

Journal

Language

English

Abstract

We have synthesized a new family of π -conjugated dendrimers that are based on bis(enediynyl)benzene units by using both divergent and convergent approaches. The compds. at all three generations have strong bluish-green fluorescence, especially the third-generation dendrimer, which has the highest extinction coefficient and quantum efficiency in this series.

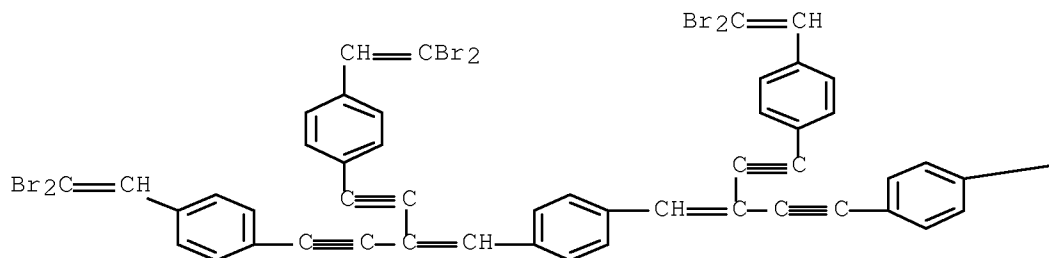
Hit Structure

CAS Registry Number
754233-15-3 CAPLUS

Chemical or Trade Name

Benzene, 1,4-bis[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

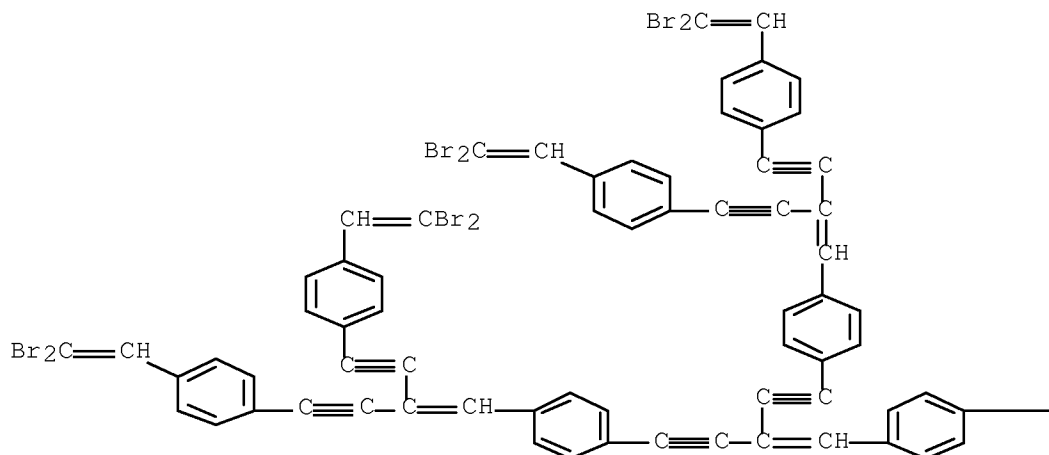


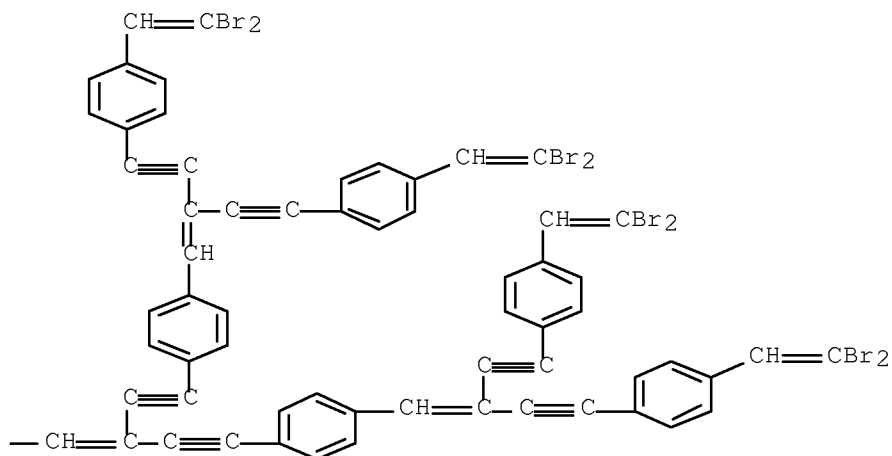
CAS Registry Number
754233-16-4 CAPLUS

Chemical or Trade Name

Benzene, 1,4-bis[4-[4-[4-(2,2-dibromoethenyl)phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]phenyl]-2-[[4-(2,2-dibromoethenyl)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

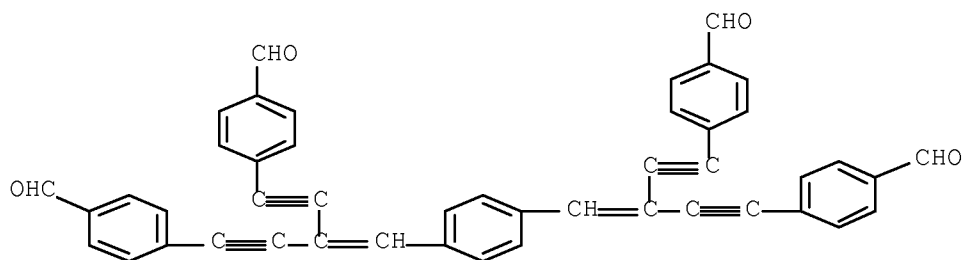
PAGE 1-A





CAS Registry Number
754233-17-5 CAPLUS

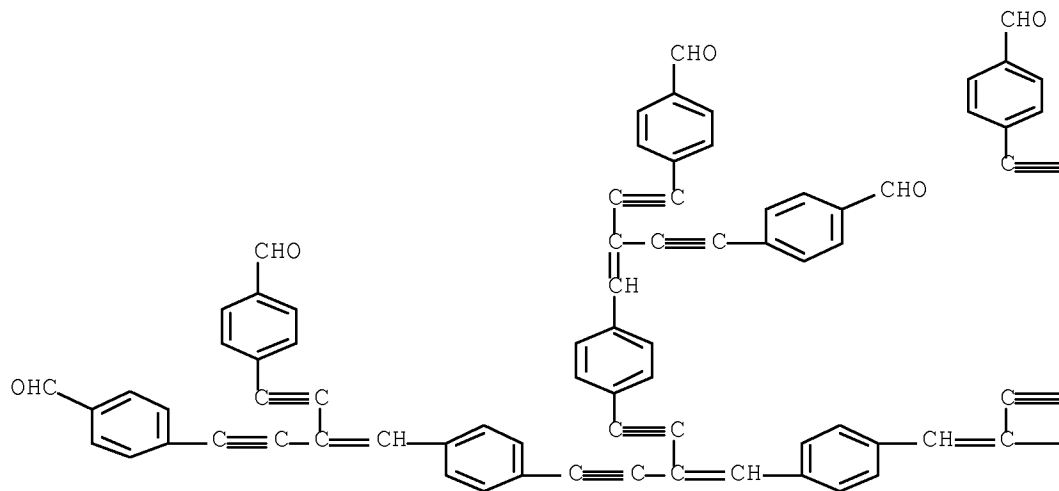
Chemical or Trade Name
Benzaldehyde, 4,4'-[[3-[[4-[4-(4-formylphenyl)-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis- (9CI) (CA INDEX NAME)



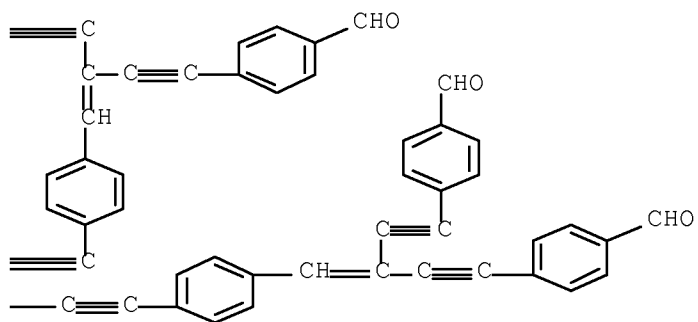
CAS Registry Number
754233-18-6 CAPLUS

Chemical or Trade Name
Benzaldehyde, 4,4'-[[3-[[4-[4-[4-(4-formylphenyl)-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]-2-[(4-formylphenyl)ethynyl]-1-buten-3-ynyl]phenyl]ethynyl]-1-buten-3-ynyl]phenyl]methylene]-1,4-pentadiyne-1,5-diyl]bis[4,1-phenylene[3-[(4-formylphenyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS RECORD (17 CITINGS)

Accession Number

2004:480115 CAPLUS [Full-text](#)

Document Number

141:190674

Title

Synthesis of Conjugated Oligomers Having Aromatic and Enediyne Units Alternately in the Backbone that Show Intense Fluorescence Emission

Author/Inventor

Nakano, Yuuki; Ishizuka, Kenichi; Muraoka, Kenji; Ohtani, Hiroyuki; Takayama, Yuuki; Sato, Fumie

Patent Assignee/Corporate Source

Department of Biomolecular Engineering, Tokyo Institute of Technology, Midori, Yokohama, Kanagawa, 226-8501, Japan

Source

Organic Letters (2004), 6(14), 2373-2376 CODEN: ORLEF7; ISSN: 1523-7060

Document Type

Journal

Language

English

Abstract

Synthesis and fluorescence properties of π -conjugated compds. I ($n = 1-3$; X = 1,4-phenylene, 2,5-pyridine, 2,5-thiophene; R = n-Pr, n-Bu) having alternately an aromatic or heteroarom. ring and an enediyne unit in the backbone are described.

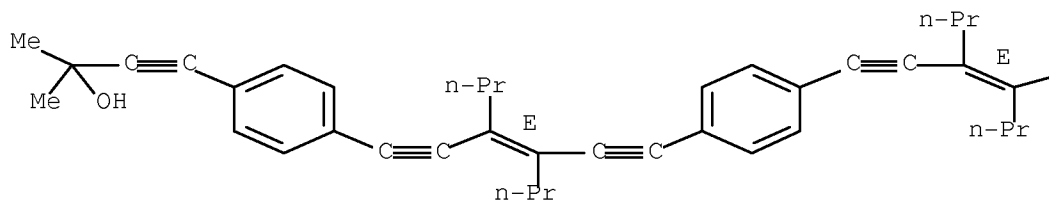
Hit Structure

CAS Registry Number
740810-62-2 CAPLUS

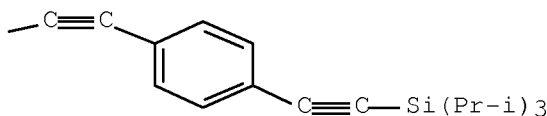
Chemical or Trade Name

3-Butyn-2-ol, 2-methyl-4-[4-[(3E)-3-propyl-4-[[4-[(3E)-3-propyl-4-[[4-[[tris(1-methylethyl)silyl]ethynyl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]- (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

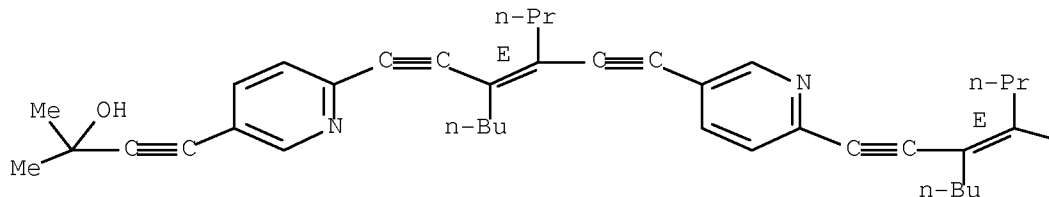


CAS Registry Number
740810-65-5 CAPLUS

Chemical or Trade Name

3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)

PAGE 1-A



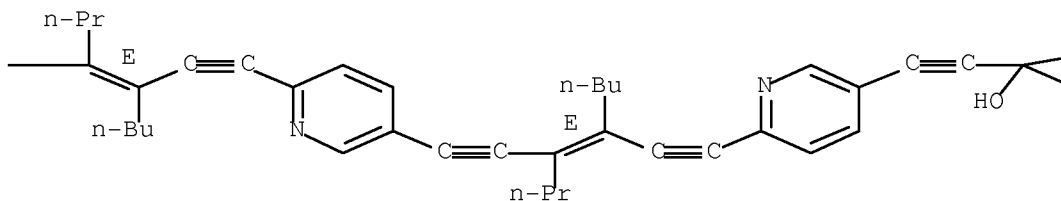
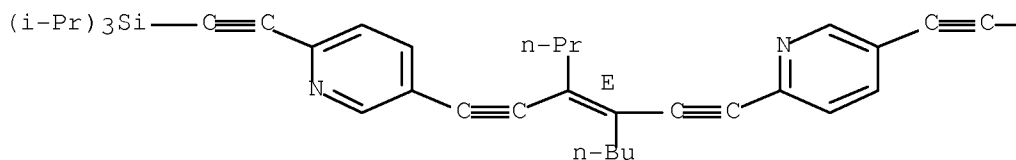
Chemical or Trade Name
3-Butyn-2-ol, 2-methyl-4-[5-[(3E)-3-propyl-4-[[5-[(3E)-3-propyl-4-[[5-
[[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-
2-thienyl]ethynyl]-3-hepten-1-yn-1-yl]-2-thienyl]- (CA INDEX NAME)

Chemical or Trade Name
3-Butyn-2-ol, 2-methyl-4-[4-{(3E)-3-propyl-4-[[4-{(3E)-3-propyl-4-[[4-(3E)-3-propyl-4-[[4-{tris(1-methylethyl)silyl]ethynyl}phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]ethynyl]-3-hepten-1-yn-1-yl]phenyl]-3-hepten-1-yn-1-yl]phenyl- (CA INDEX NAME)



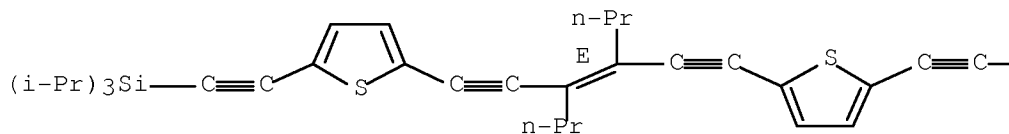
CAS Registry Number
740810-66-6 CAPLUS

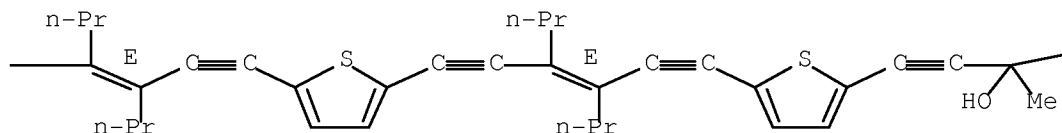
Chemical or Trade Name
3-Butyn-2-ol, 4-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[(3E)-3-butyl-4-[2-[6-[[tris(1-methylethyl)silyl]ethynyl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]ethynyl]-3-hepten-1-yn-1-yl]-3-pyridinyl]-2-methyl- (CA INDEX NAME)



CAS Registry Number
740810-69-9 CAPLUS

Chemical or Trade Name
3-Butyn-2-ol, 4-[5-[[(3E)-4-[2-[5-[[(3E)-5-ethyl-4-[2-[5-[[(3E)-5-ethyl-3-propyl-4-[2-[5-[2-[tris(1-methylethyl)silyl]ethynyl]-2-thienyl]ethynyl]-3-penten-1-yn-1-yl]-2-thienyl]ethynyl]-3-propyl-3-hepten-1-yn-1-yl]-2-thienyl]-2-methyl- (CA INDEX NAME)





OS.CITING REF COUNT: 23 THERE ARE 23 CAPLUS RECORDS THAT CITE THIS RECORD (24 CITINGS)

.L8 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2004:328526 CAPLUS [Full text](#)

Document Number

141:54000

Title

Solid-phase synthesis of oligo(triacetylene)s and oligo(phenylenetriacetylene)s employing Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions

Author/Inventor

Utesch, Nils F.; Diederich, Francois; Boudon, Corinne; Gisselbrecht, Jean-Paul; Gross, Maurice

Patent Assignee/Corporate Source

Laboratorium fuer Organische Chemie, ETH-Hoenggerberg, HCI, Zurich, CH-8093, Switz.

Source

Helvetica Chimica Acta (2004), 87(3), 698-718 CODEN: HCACAV; ISSN: 0018-019X

Document Type

Journal

Language

English

Abstract

The polymer-supported synthesis of poly(triacetylene)-derived monodisperse oligomers is described, using Pd0-catalyzed Sonogashira and Cadiot-Chodkiewicz-type cross-couplings as the key steps in the construction of the acetylenic scaffolds. Merrifield resin functionalized with a 1-(4-iodoaryl)triazene linker was chosen as the polymeric support. The linker selection was made based on the results of several model studies in the liquid phase. For the solid-support synthesis of p-[C6H4C.tpbond.CC(CH2OSiMe2CMe3);C(CH2OSiMe2CMe3)C.tpbond.C]nSiMe3 [I, n = 2-4] a set of only three reactions was required: (i) Pd0-catalyzed Sonogashira cross-coupling, (ii) Me3Si-alkyne deprotection by protodesilylation, and (iii) cleavage of the linker with liberation of I. The longest-wavelength absorption maxima of I [n = 1-4] shift bathochromically with increasing oligomeric length, from λ_{max} 337 nm (I, n = 1) to 384 nm (I, n = 4). Based on the electronic absorption data, the effective conjugation length (ECL) of the oligo(phenylene triacetylene)s is estimated to involve at least four monomer units and 40 C-atoms. π -Electron conjugation in these oligomers is less efficient than in Me3Si[C6H4C.tpbond.CC(CH2OSiMe2CMe3);C(CH2OSiMe2CMe3)C.tpbond.C]nSiMe3 (II) due to poor transmittance of π -electron delocalization by the Ph rings inserted into the oligomeric backbone. Similar conclusions were drawn from the electrochem. properties of the two oligomeric series as determined by cyclic (CV) and rotating-disk voltammetry. In sharp contrast to II, I are strongly fluorescent, with the highest quantum yield Φ_F = 0.69 measured for I [n = 3]. Whereas the Sonogashira cross-coupling on solid support proceeded smoothly, optimal conditions for alkyne-alkyne cross-coupling reactions employing Pd0-catalyzed Cadiot-Chodkiewicz conditions still remain to be developed.

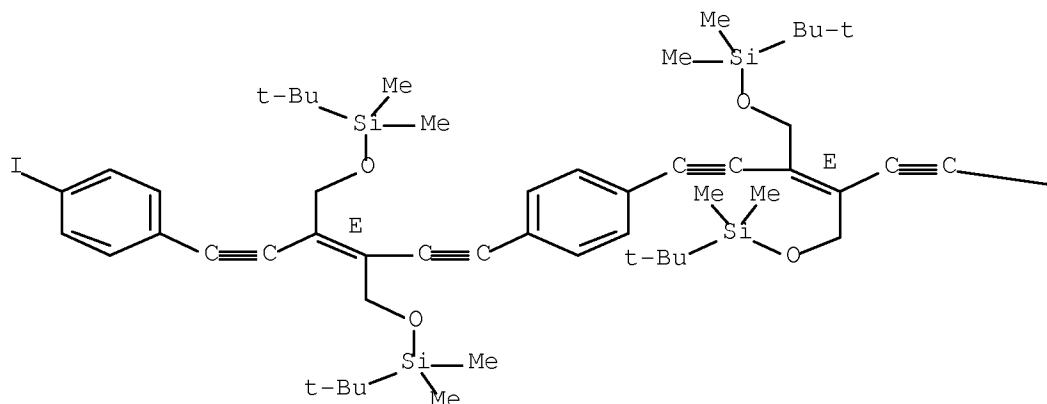
Hit Structure

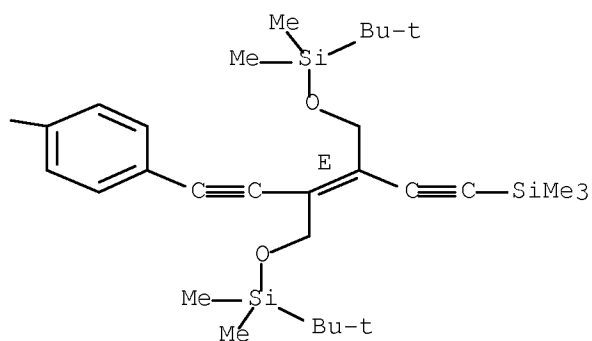
CAS Registry Number

554459-63-1 CAPLUS

Chemical or Trade Name

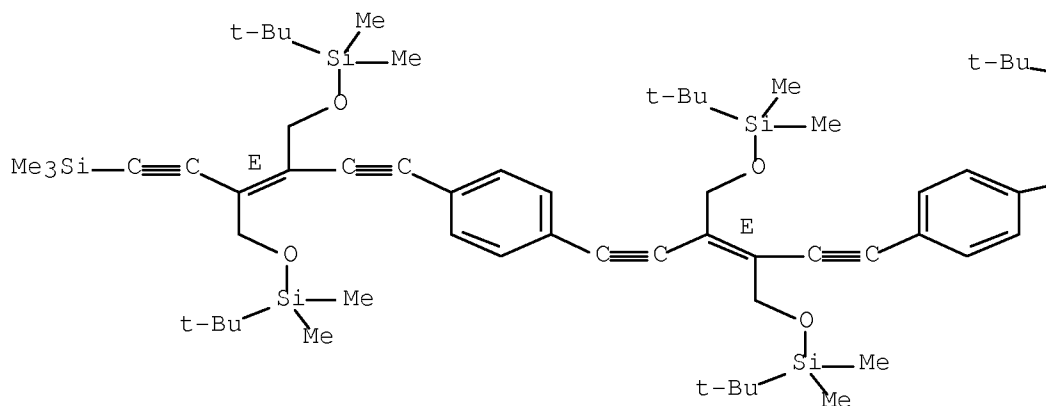
4,9-Dioxa-3,10-disiladodeco-6-ene, 6-[[4-[(3E)-6-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-7-[(trimethylsilyl)ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

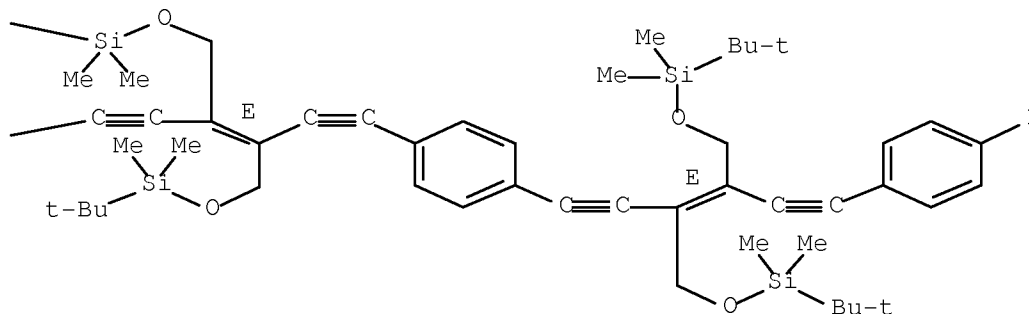




CAS Registry Number
554459-64-2 CAPLUS

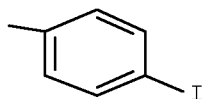
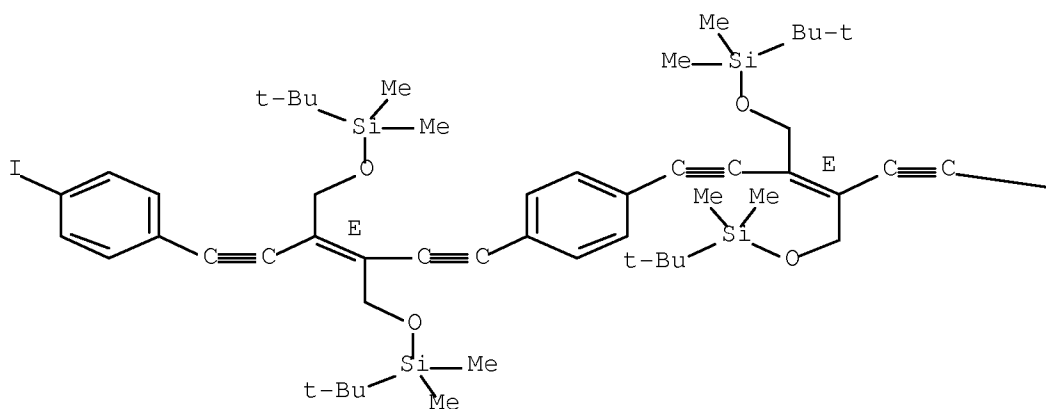
Chemical or Trade Name
4,9-Dioxo-3,10-disiladodeco-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)





CAS Registry Number
704916-29-0 CAPLUS

Chemical or Trade Name
4,9-Dioxaspiro[3.10]undec-6-ene, 6,6'-(1,4-phenylenedi-2,1-ethynediyl)bis[7-[(4-iodophenyl)ethynyl]-2,2,3,3,10,10,11,11-octamethyl-, (6E,6'E)-(9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 8 THERE ARE 8 CAPLUS RECORDS THAT CITE THIS RECORD
(8 CITINGS)

, L8 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2003:827385 CAPLUS [Full-text](#)

Document Number

140:59755

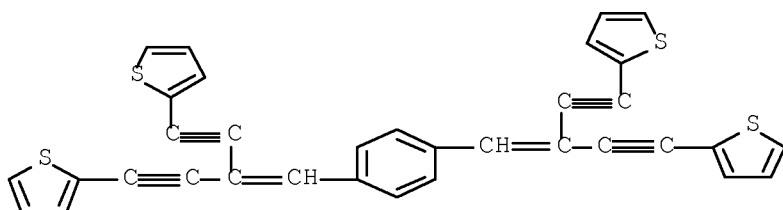
Title

Synthesis and reactivity of dinuclear rhodium complexes with Rh:C:CHR and Rh:C:C:RRR' units as building blocks

Author/Inventor

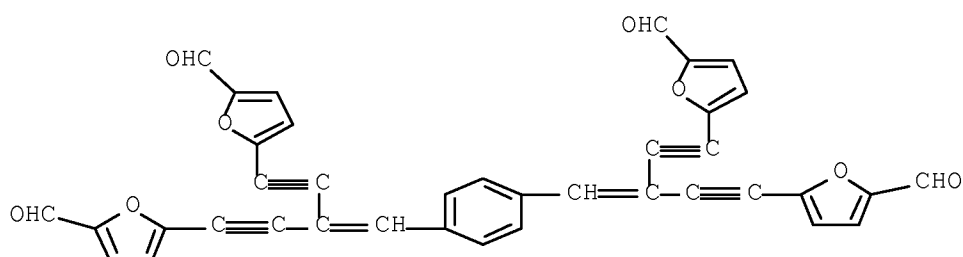
Chemical or Trade Name

Thiophene, 2,2'-[1,4-phenylenebis[3-(2-thienylethynyl)-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



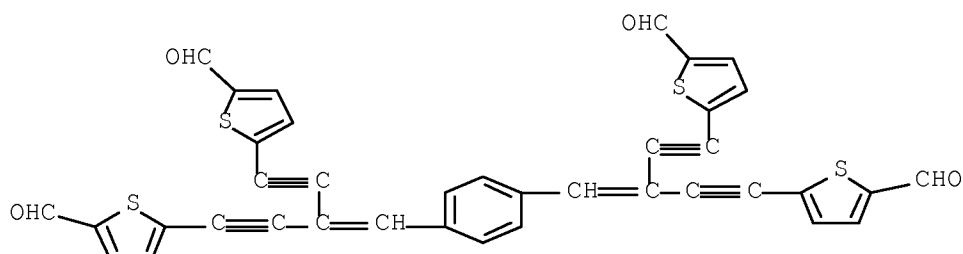
CAS Registry Number
360549-91-3 CAPLUS

Chemical or Trade Name
2-Furancarboxaldehyde, 5,5'-[1,4-phenylenebis[3-[(5-formyl-2-furanyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



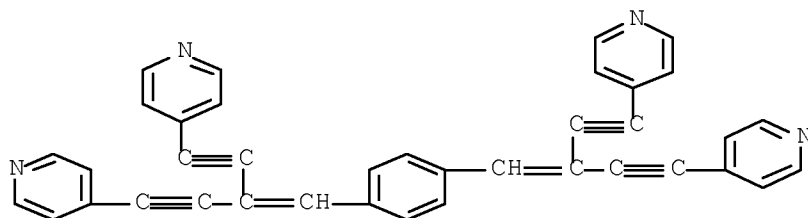
CAS Registry Number
360549-92-4 CAPLUS

Chemical or Trade Name
2-Thiophenecarboxaldehyde, 5,5'-[1,4-phenylenebis[3-[(5-formyl-2-thienyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



CAS Registry Number
360549-93-5 CAPLUS

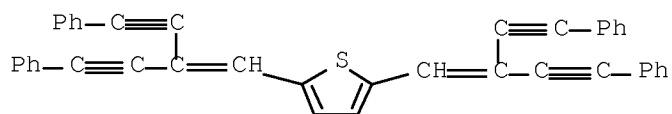
Chemical or Trade Name
Pyridine, 4,4'-[1,4-phenylenebis[3-(4-pyridylethynyl)-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



CAS Registry Number

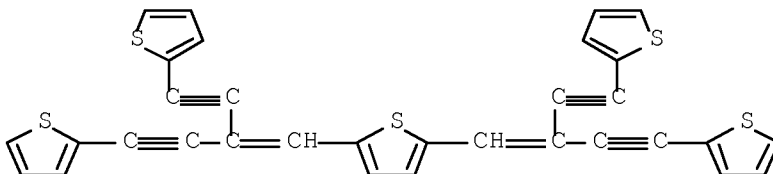
360549-94-6 CAPLUS

Chemical or Trade Name
Thiophene, 2,5-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



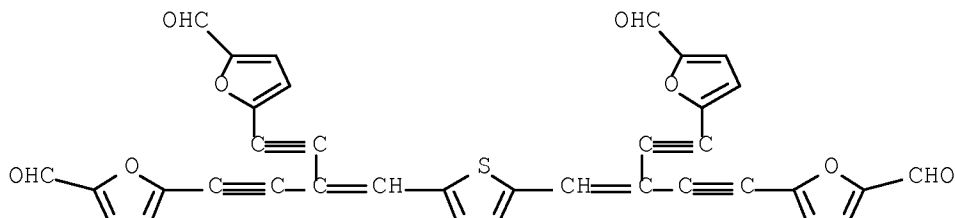
CAS Registry Number
360549-95-7 CAPLUS

Chemical or Trade Name
Thiophene, 2,5-bis[4-(2-thienyl)-2-[2-(2-thienyl)ethynyl]-1-buten-3-yn-1-yl]- (CA INDEX NAME)



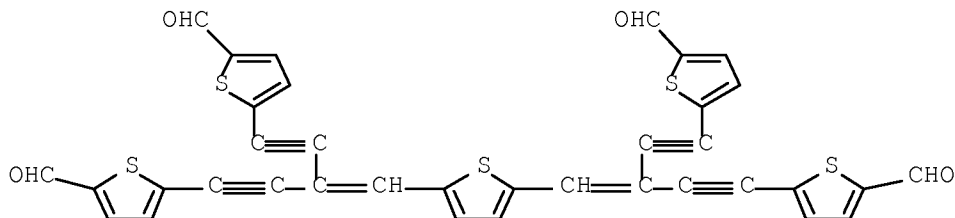
CAS Registry Number
360549-96-8 CAPLUS

Chemical or Trade Name
2-Furancarboxaldehyde, 5,5'-[2,5-thiophenediylbis[3-[(5-formyl-2-furanyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



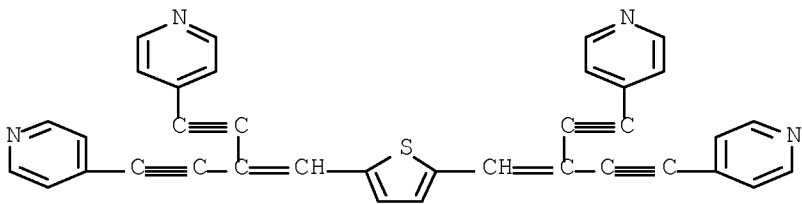
CAS Registry Number
360549-97-9 CAPLUS

Chemical or Trade Name
2-Thiophenecarboxaldehyde, 5,5'-[2,5-thiophenediylbis[3-[(5-formyl-2-thienyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



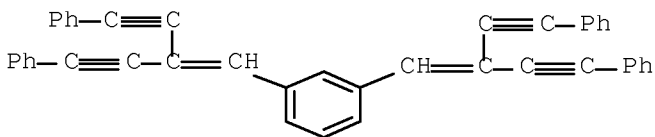
CAS Registry Number
360549-98-0 CAPLUS

Chemical or Trade Name
Pyridine, 4,4'-[2,5-thiophenediylbis[3-(4-pyridinylethynyl)-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



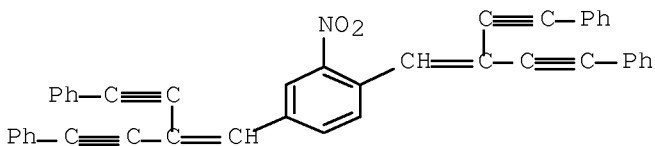
CAS Registry Number
610283-06-2 CAPLUS

Chemical or Trade Name
Benzene, 1,3-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



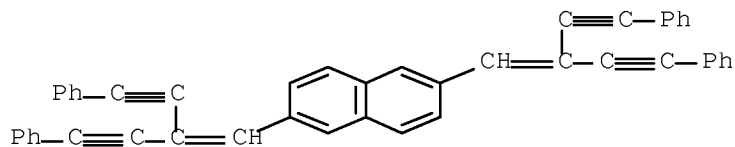
CAS Registry Number
610283-08-4 CAPLUS

Chemical or Trade Name
Benzene, 2-nitro-1,4-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



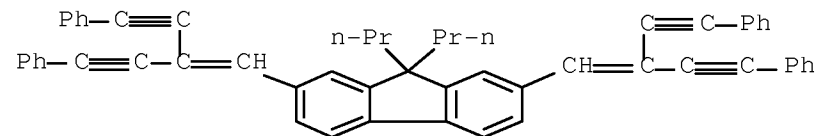
CAS Registry Number
610283-09-5 CAPLUS

Chemical or Trade Name
Naphthalene, 2,6-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



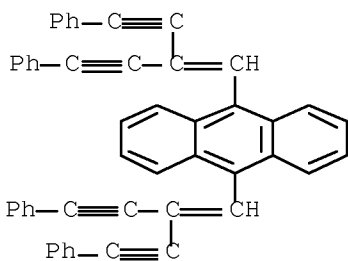
CAS Registry Number
610283-10-8 CAPLUS

Chemical or Trade Name
9H-Fluorene, 2,7-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]-9,9-dipropyl- (CA INDEX NAME)



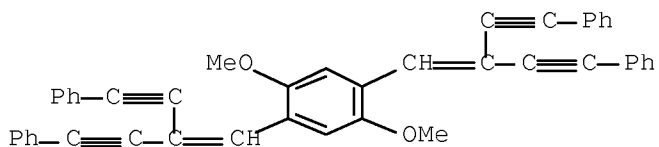
CAS Registry Number
610283-11-9 CAPLUS

Chemical or Trade Name
Anthracene, 9,10-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



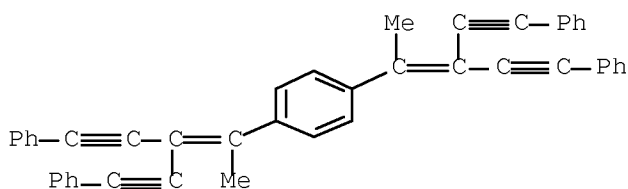
CAS Registry Number
610283-12-0 CAPLUS

Chemical or Trade Name
Benzene, 1,4-dimethoxy-2,5-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



CAS Registry Number
610283-13-1 CAPLUS

Chemical or Trade Name
Benzene, 1,4-bis[1-methyl-4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



OS.CITING REF COUNT: 49 THERE ARE 49 CAPLUS RECORDS THAT CITE THIS
RECORD (49 CITINGS)

Accession Number

2003:424686 CAPLUS [Full-text](#)

Document Number

139:150012

Title

Synthesis of Highly Fluorescent Y-Enyne Dendrimers with Four and Six Arms

Author/Inventor

Kaafarani, Bilal R.; Wex, Brigitte; Wang, Fei; Catanesu, Otilia; Chien, L. C.; Neckers, Douglas C.

Patent Assignee/Corporate Source

Center for Photochemical Sciences, Bowling Green State University, Bowling Green, OH, 43403, USA

Source

Journal of Organic Chemistry (2003), 68(13), 5377-5380 CODEN: JOCEAH; ISSN: 0022-3263

Document Type

Journal

Language

English

Abstract

A first generation of dendrimeric Y-enynes with extended flexible chains was synthesized using Sonogashira coupling. Dendrimers 9 and 10 are highly fluorescent in the solid state and in solution

Hit Structure

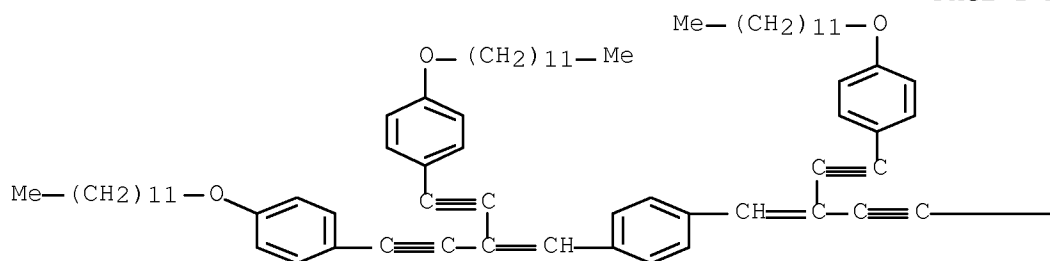
CAS Registry Number

569670-22-0 CAPLUS

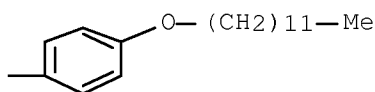
Chemical or Trade Name

Benzene, 1,4-bis[4-[4-(dodecyloxy)phenyl]-2-[[4-(dodecyloxy)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

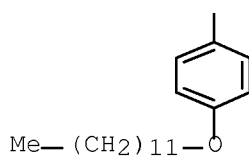
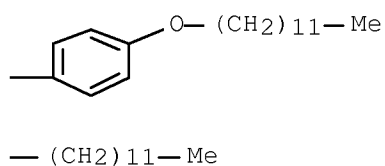
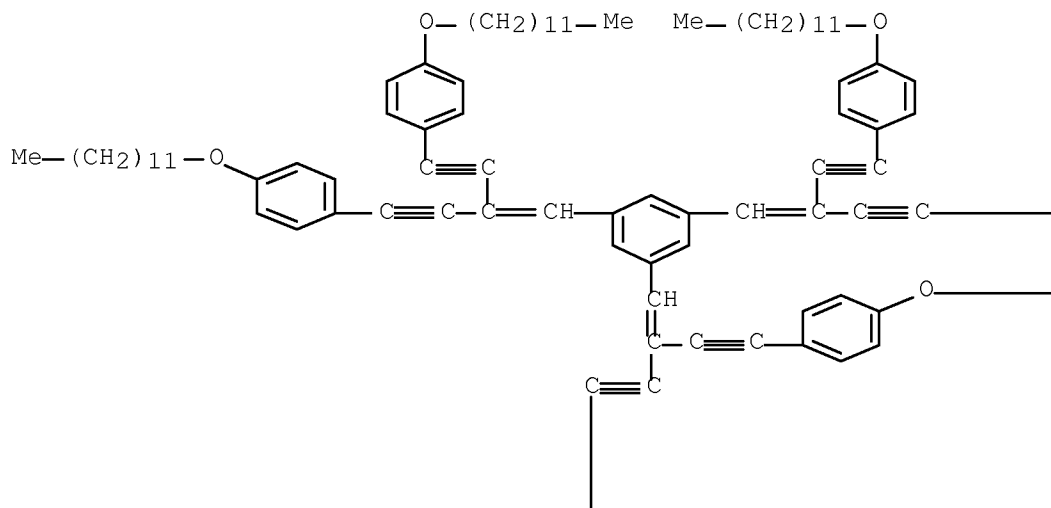


CAS Registry Number

569670-23-1 CAPLUS

Chemical or Trade Name

Benzene, 1,3,5-tris[4-[4-(dodecyloxy)phenyl]-2-[[4-(dodecyloxy)phenyl]ethynyl]-1-buten-3-ynyl]- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS RECORD (17 CITINGS)

, L8 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2003:234291 CAPLUS [Full-text](#)

Document Number

139:85055

Title

Acetylenic scaffolding on solid support: Poly(triacetylene)-derived oligomers by Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions

Author/Inventor

Utesch, Nils F.; Diederich, Francois

Patent Assignee/Corporate Source

Laboratorium fur Organische Chemie, ETH-Honggerberg, HCI, Zurich, CH-8093, Switz.

Source

Organic & Biomolecular Chemistry (2003), 1(2), 237-239 CODEN: OBCRAK; ISSN: 1477-0520

Document Type

Journal

Language

English

Abstract

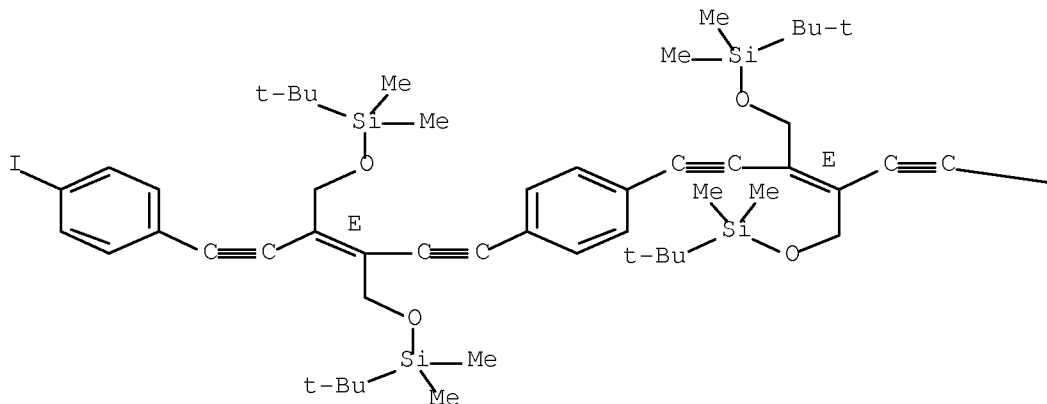
Synthesis of poly(triacetylene)-derived oligomers by Pd(0)-catalyzed Sonogashira and Cadiot-Chodkiewicz-type cross-coupling reactions on solid support is reported. Oligo(phenylene triacetylene)s, e.g., [4-C6H4C.tpbond.CCR.CRC.tpbond.C]nSiMe3 (R = CH2OSiButMe2, n = 1, 2, 3, 4) members of a new class of linearly π-conjugated oligomers with all-C backbones, feature very high fluorescence intensities.

Hit Structure

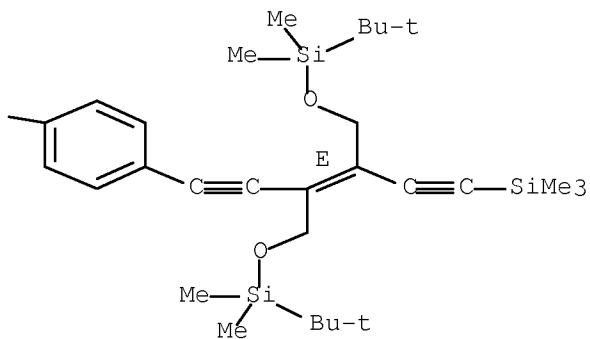
CAS Registry Number
554459-63-1 CAPLUS

Chemical or Trade Name
4,9-Dioxo-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,10,10,11,11-octamethyl-7-[[trimethylsilyl]ethynyl]-, (6E)- (9CI) (CA INDEX NAME)

PAGE 1-A



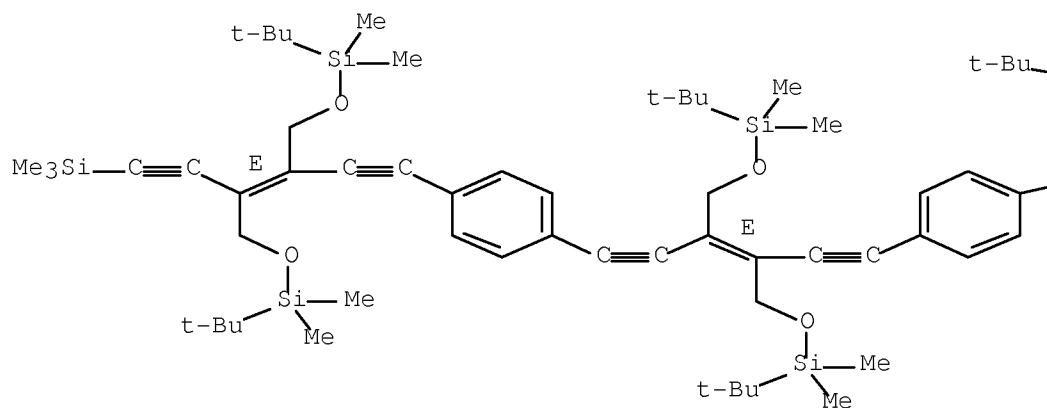
PAGE 1-B



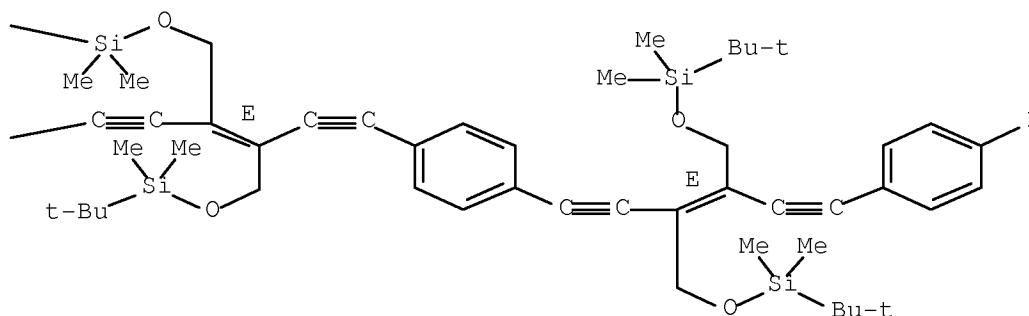
CAS Registry Number
554459-64-2 CAPLUS

Chemical or Trade Name
4,9-Dioxo-3,10-disiladodec-6-ene, 6-[[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(4-iodophenyl)-3-hexene-1,5-diynyl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diynyl]phenyl]ethynyl]-7-[[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diynyl]phenyl]ethynyl]-2,2,3,10,10,11,11-octamethyl-, (6E)- (9CI) (CA INDEX NAME)

PAGE 1-A



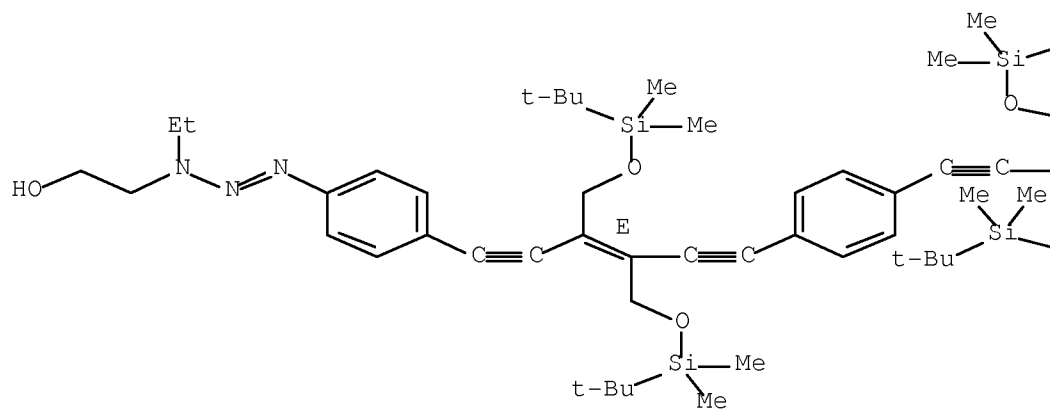
PAGE 1-B

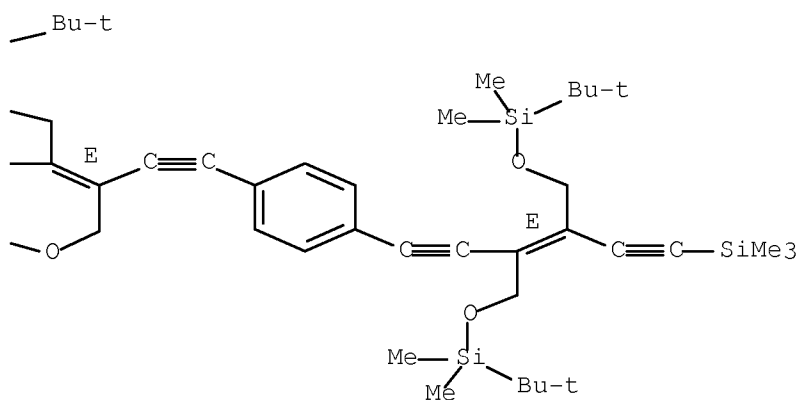


CAS Registry Number
554459-72-2 CAPLUS

Chemical or Trade Name
Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazen-1-yl]- (CA INDEX NAME)

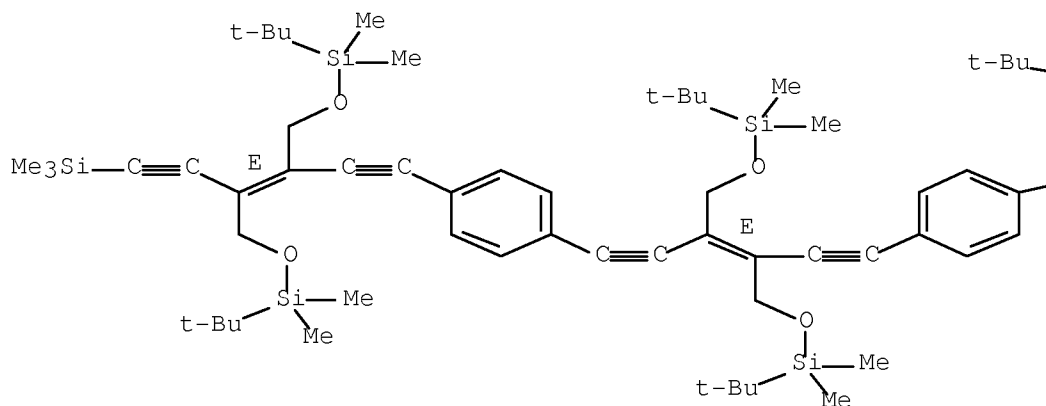
PAGE 1-A

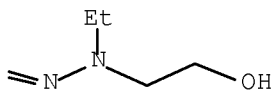
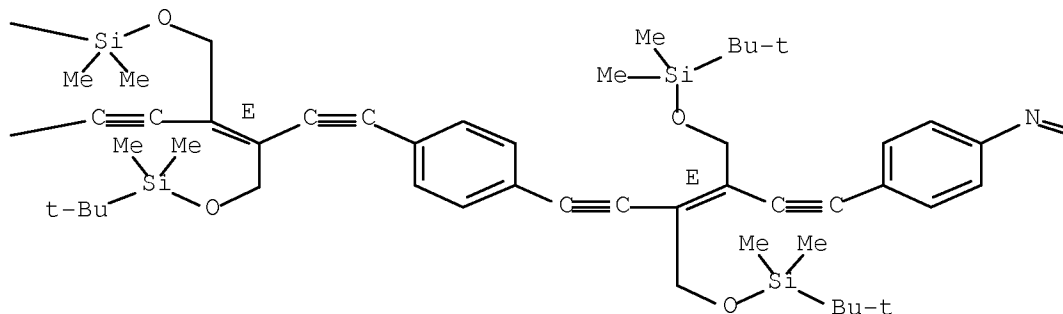




CAS Registry Number
554459-73-3 CAPLUS

Chemical or Trade Name
Ethanol, 2-[3-[4-[(3E)-6-[4-[(3E)-6-[4-[(3E)-6-[4-[(3E)-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-6-(trimethylsilyl)-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-3,4-bis[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3-hexene-1,5-diyn-1-yl]phenyl]-1-ethyl-2-triazen-1-yl]- (CA INDEX NAME)





OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (19 CITINGS)

L8 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2001:714296 CAPLUS [Full-text](#)

Document Number

136.69640

Title

Synthesis and spectroscopic studies of expanded planar dehydrotribenzo[n]annulenes containing one or two isolated alkene units

Author/Inventor

Wan, W. Brad; Chiechi, Ryan C.; Weakley, Timothy J. R.; Haley, Michael M.

Patent Assignee/Corporate Source

Department of Chemistry and the Materials Science Institute, University of Oregon, Eugene, OR, 97403-1253, USA

Source

European Journal of Organic Chemistry (2001), (18), 3485-3490 CODEN: EJOCFK; ISSN: 1434-193X

Document Type

Journal

Language

English

Abstract

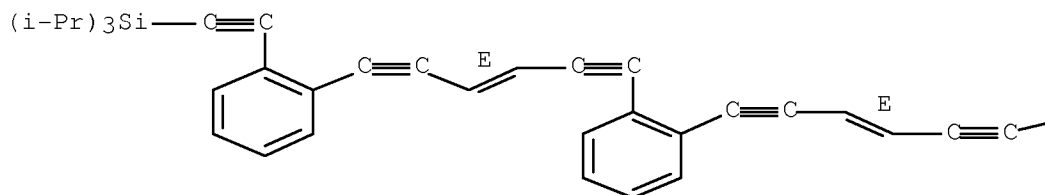
Dehydrobenzoannulene derivs. containing isolated alkene linkages, e.g., I, were synthesized by combining an in situ Pd/Cu-mediated cross-coupling with an intramol. cyclization strategy. ¹H NMR studies of these macrocycles and comparison with related systems verify that highly alkynylated dehydrobenzoannulenes possess weak induced ring currents, indicative of aromatic (4n+2 π systems) and antiarom. (4n π systems) behavior, in spite of their large size and extensive benzannulation.

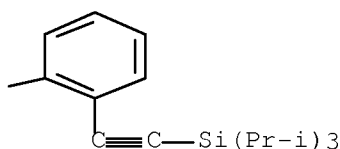
Hit Structure

CAS Registry Number
383404-38-4 CAPLUS

Chemical or Trade Name

Silane, [1,2-phenylenebis[(3E)-3-hexene-1,5-diyne-6,1-diyl-2,1-phenylene-2,1-ethynediyl]]bis[tris(1-methylethyl)- (9CI) (CA INDEX NAME)





OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

.L8 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2001:519766 CAPLUS [Full-text](#)

Document Number

135:243732

Title

Novel fluorophores: efficient synthesis and photophysical study

Author/Inventor

Hwang, Gil Tae; Son, Hyung Su; Ku, Ja Kang; Kim, Byeang Hyeon

Patent Assignee/Corporate Source

Center for Integrated Molecular Systems Department of Chemistry Division of Molecular Life Science, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

Source

Organic Letters (2001), 3(16), 2469-2471 CODEN: ORLEF7; ISSN: 1523-7060

Document Type

Journal

Language

English

Abstract

We have synthesized novel tetraacetylenic fluorophores by using Sonogashira reactions of 1,4-bis(dibromovinyl)benzene and 2,5-bis(dibromovinyl)thiophene with various aromatic bromides. The emission maxima of these fluorophores vary from the indigo blue to the reddish-orange region, depending on the structures of the aromatic nuclei and peripheral moieties.

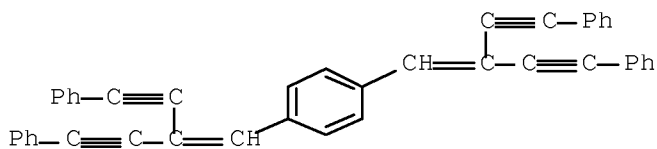
Hit Structure

CAS Registry Number

360549-89-9 CAPLUS

Chemical or Trade Name

Benzene, 1,4-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)

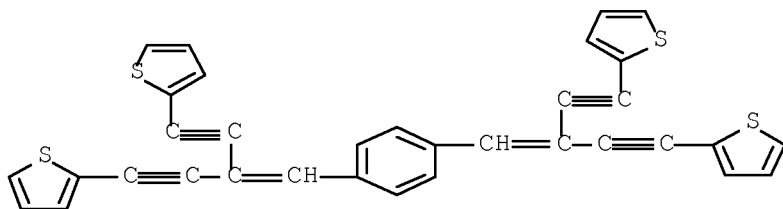


CAS Registry Number

360549-90-2 CAPLUS

Chemical or Trade Name

Thiophene, 2,2'-[1,4-phenylenebis[3-(2-thienylethynyl)-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)

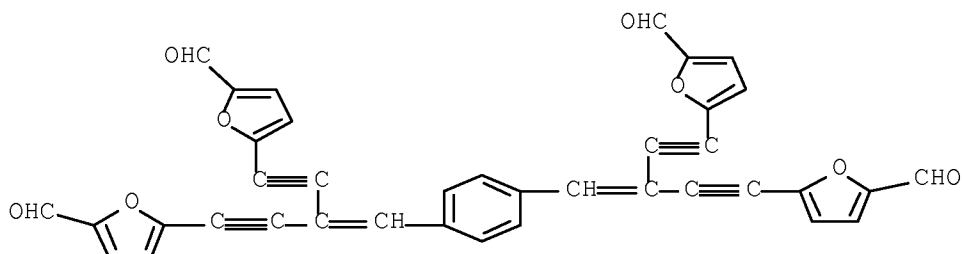


CAS Registry Number

360549-91-3 CAPLUS

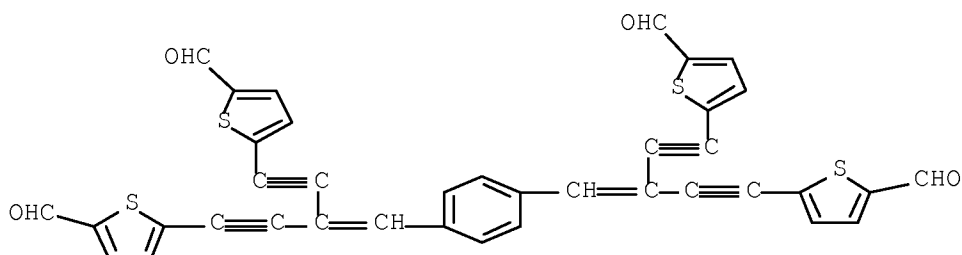
Chemical or Trade Name

2-Furancarboxaldehyde, 5,5'-[1,4-phenylenebis[3-[(5-formyl-2-furanyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



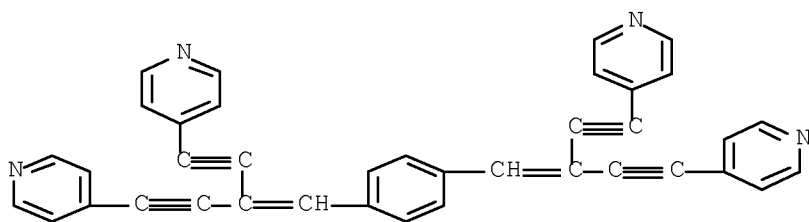
CAS Registry Number
360549-92-4 CAPLUS

Chemical or Trade Name
2-Thiophenecarboxaldehyde, 5,5'-[1,4-phenylenebis[3-[(5-formyl-2-thienyl)ethynyl]-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



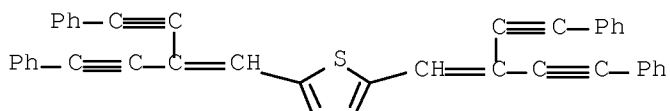
CAS Registry Number
360549-93-5 CAPLUS

Chemical or Trade Name
Pyridine, 4,4'-[1,4-phenylenebis[3-(4-pyridinylethynyl)-3-buten-1-yne-4,1-diyl]]bis- (9CI) (CA INDEX NAME)



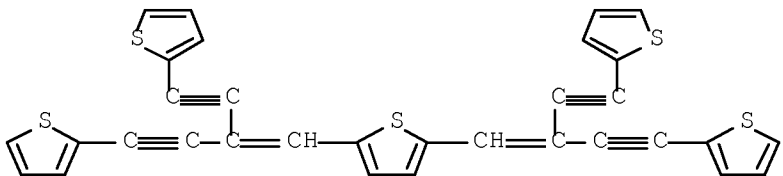
CAS Registry Number
360549-94-6 CAPLUS

Chemical or Trade Name
Thiophene, 2,5-bis[4-phenyl-2-(2-phenylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



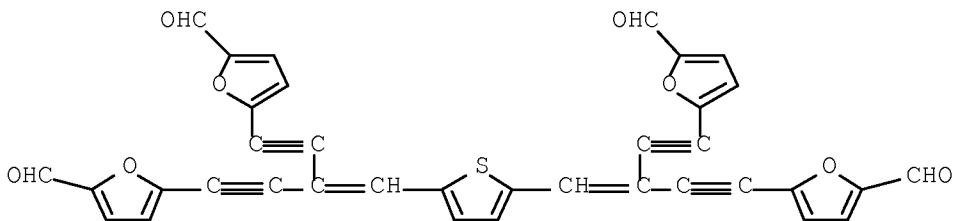
CAS Registry Number
360549-95-7 CAPLUS

Chemical or Trade Name
Thiophene, 2,5-bis[4-(2-thienyl)-2-(2-thienylethynyl)-1-buten-3-yn-1-yl]- (CA INDEX NAME)



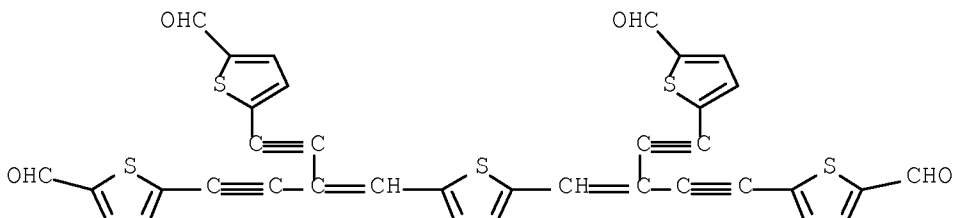
CAS Registry Number
360549-96-8 CAPLUS

Chemical or Trade Name
2-Furancarboxaldehyde, 5,5'-[2,5-thiophenediylbis[3-[(5-Formyl-2-furanyl)ethynyl]-3-buten-1-yne-4,1-diy]]bis- (9CI) (CA INDEX NAME)



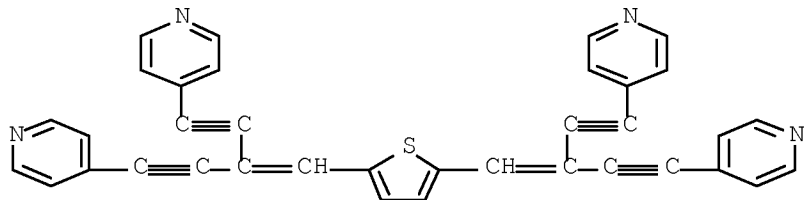
CAS Registry Number
360549-97-9 CAPLUS

Chemical or Trade Name
2-Thiophenecarboxaldehyde, 5,5'-[2,5-thiophenediylbis[3-[(5-formyl-2-thienyl)ethynyl]-3-buten-1-yne-4,1-diy]]bis- (9CI) (CA INDEX NAME)



CAS Registry Number
360549-98-0 CAPLUS

Chemical or Trade Name
Pyridine, 4,4'-[2,5-thiophenediylbis[3-(4-pyridinylethynyl)-3-buten-1-yne-4,1-diy]]bis- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 27 THERE ARE 27 CAPLUS RECORDS THAT CITE THIS RECORD (27 CITINGS)

L8 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number
1996:29553 CAPLUS [Full-text](#)

Document Number
124:260436

Title
Synthesis and reactions of new ethynyl-substituted 1,6-methano[10]annulenes

Author/Inventor
Bryant-Freidrich, Amanda; Neidlein, Richard

Patent Assignee/Corporate Source
Pharm.-Chem. Inst., Univ. Heidelberg, Heidelberg, D-69120, Germany

Source
Synthesis (1995), (12), 1506-10 CODEN: SYNTBF; ISSN: 0039-7881

Document Type
Journal

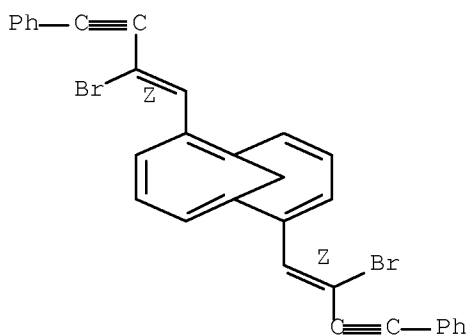
Language
English

Abstract
Stereospecific Pd(PPh₃)₄ catalyzed coupling of an acetylene to geminal dibromo-substituted alkenes yielded enynes, which upon dehydrohalogenation formed butadiynyl substituted 1,6-methano[10]annulenes I [R = (C.tplbond.C)2R3; R1 = R2 = H, R3 = Ph, CMe3; R1 = H, R = R2 = (C.tplbond.C)2Ph; R = R1 = (C.tplbond.C)2Ph, R2 = H].

Hit Structure

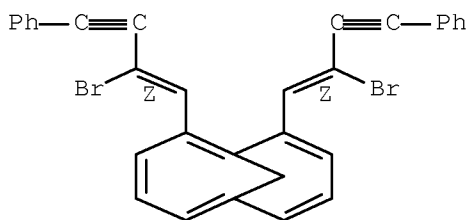
CAS Registry Number
175430-09-8 CAPLUS

Chemical or Trade Name
Bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene,
2,7-bis(2-bromo-4-phenyl-1-buten-3-ynyl)-, (Z,Z)- (9CI) (CA INDEX NAME)



CAS Registry Number
175430-11-2 CAPLUS

Chemical or Trade Name
Bicyclo[4.4.1]undeca-1,3,5,7,9-pentaene,
2,10-bis(2-bromo-4-phenyl-1-buten-3-ynyl)-, (Z,Z)- (9CI) (CA INDEX NAME)



L8 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number
1994:192448 CAPLUS [Full-text](#)

Document Number
120:192448

Title
Synthesis of a series of conjugated enyne polythiophenes

Author/Inventor
Kane, James J.; Gao, Feng; Reinhardt, Bruce A.; Evers, Robert C.

Patent Assignee/Corporate Source
Chem. Dep., Wright State Univ., Dayton, OH, 45435-0001, USA

Source
Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) (1992), 33(1), 1064-5 CODEN: ACPPAY; ISSN: 0032-3934

Document Type
Journal

Language
English

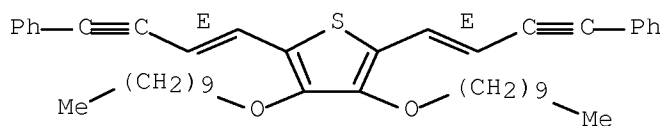
Abstract
The title polymers were prepared via polymerization of 3,4-didecyloxy-2,5-bis-(β-bromoethenyl)thiophene and aromatic diethynyl compds. Thermal and viscosity of the resulting thiophene-containing polyacetylenes are discussed.

Hit Structure

CAS Registry Number
153846-90-3 CAPLUS

Chemical or Trade Name

Thiophene, 3,4-bis(decyloxy)-2,5-bis(4-phenyl-1-buten-3-ynyl)-, (E,E)-
(9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

. L8 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1984:23114 CAPLUS [Full-Text](#)

Document Number

100:23114

Title

Cis-Enyne aromatic and aromatic heterocyclic polymers

Author/Inventor

Reinhart, Bruce

Patent Assignee/Corporate Source

United States Dept. of the Air Force, USA

Source

U. S. Pat. Appl., 4 pp. Avail. NTIS Order No. PAT-APPL-6-399 661. CODEN: XAXXAV

Document Type

Patent

Language

English

Patent Information

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 399661	A0	19830304	US 1982-399661	19820719
US 4417039	A	19831122		

Abstract

Aromatic and aromatic heterocyclic enyne polymers having relatively low glass temps. for fabrication are prepared by treating 1,4-bis(cis-β-bromovinyl)benzene (I) [88248-70-8] with a diacetylenic compound. The polymers exhibit high glass temps. and low solvent susceptibilities after heat treatment. Thus, a suspension of 40 g p-phenylenediacrylic acid [16323-43-6] in 300 g Br was stirred for 3 h to give β,β'-p-phenylenebis(α,β-dibromopropionic acid) (II) [88248-71-9]. A mixture of 21.5 g II and 20.0 g NaHCO₃ in 500 mL acetone was refluxed for 72 h to give I. A mixture of 0.5 g I and 0.7658 g 4,4'-bis(3-ethynylphenoxy)diphenyl sulfone [63770-82-1] was dissolved in a solution of 3 mL Et₃N and 3 mL N,N-dimethylacetamide (III). A mixture of 0.025 g CuI and 0.05 g (Ph₃P)₂PdCl₂ was added. The mixture was stirred at room temperature for 70 h. Addnl. 10 mL III was added to give a polymer having glass temperature 143°. The polymer [88249-72-3] treated at 250° for 6 h had glass temperature >375° and was insol. in solvents.

Hit Structure

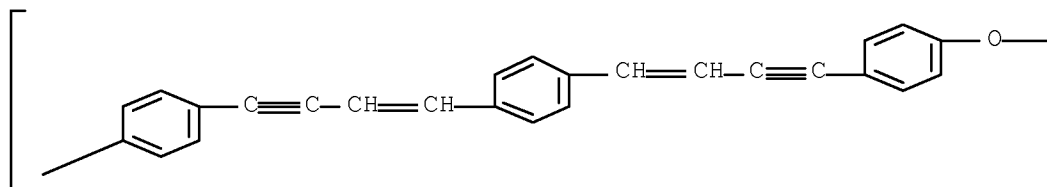
CAS Registry Number

88249-70-1 CAPLUS

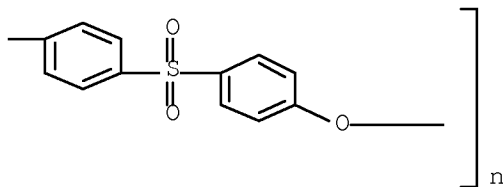
Chemical or Trade Name

Poly(oxy-1,4-phenylenesulfonyl-1,4-phenyleneoxy-1,4-phenylene-3-buten-1-yne-1,4-diyl-1,4-phenylene-1-buten-3-yne-1,4-diyl-1,4-phenylene), (Z,Z)-
(9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



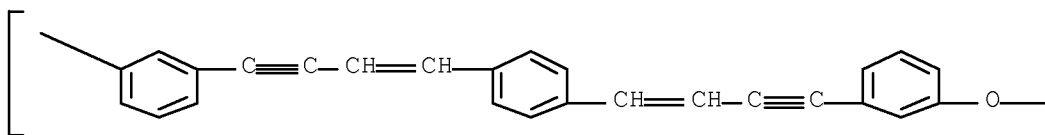
CAS Registry Number

88249-71-2 CAPLUS

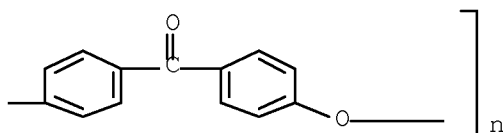
Chemical or Trade Name

Poly(oxy-1,4-phenylenecarbonyl-1,4-phenyleneoxy-1,3-phenylene-3-buten-1-yne-1,4-diyl-1,4-phenylene-1-buten-3-yne-1,4-diyl-1,3-phenylene), (Z,Z)-
(9CI) (CA INDEX NAME)

PAGE 1-A



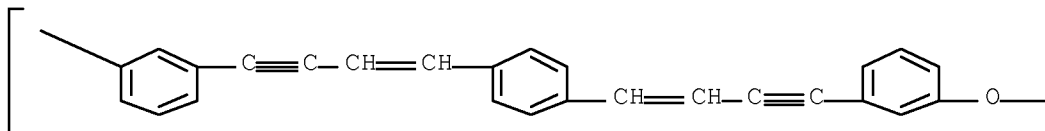
PAGE 1-B



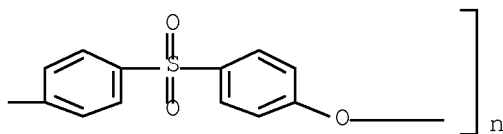
CAS Registry Number
88249-72-3 CAPLUS

Chemical or Trade Name
Poly(oxy-1,4-phenylenesulfonyl-1,4-phenyleneoxy-1,3-phenylene-3-buten-1-
yne-1,4-diyl-1,4-phenylene-1-buten-3-yne-1,4-diyl-1,3-phenylene), (Z,Z)-
(9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

L8 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1981:175327 CAPLUS Full-text

Document Number

94:175327

Title

Reactions with phosphinealkynes. XXXIX. New methods for the preparation of 1-bromoacetylenes and aromatic and conjugated enynes

Author/Inventor

Bestmann, Hans Juergen; Frey, Herbert

Patent Assignee/Corporate Source

Inst. Org. Chem., Univ. Erlangen-Nuernberg, Erlangen, D-8520, Fed. Rep. Ger.

Source

Liebigs Annalen der Chemie (1980), (12), 2061-71 CODEN: LACHDL; ISSN: 0170-2041

Document Type

Journal

Language

German

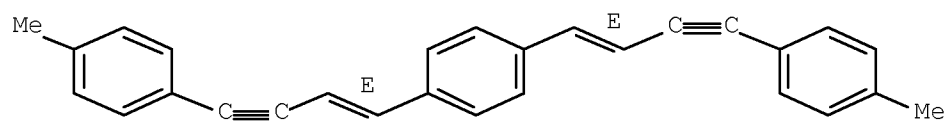
Abstract

Some of RCH:CBR₂ (R = optionally substituted Ph, naphthyl, 9-anthryl, 2-thienyl, alkyl, cycloalkyl, MeCH:CMc, MeCH:CH, MeCH:CHCH:CH, Me₂C:CHCH₂CH₂CMc:CH, retinyl, 2-furyl, PhCH:CH, PhCH:CMc), prepared in 23-85% yields from RCHO, PPh₃ and CBr₄, were dehydrobrominated with (PhCH₂)Me₃N+OH- to give 35-80% RC:lpbond.CBr (R = optionally substituted Ph, naphthyl, 9-anthryl, alkyl, cycloalkyl), which were treated with Ph₃P+MeBr- and R1CHO [R1 = 4-O₂NC₆H₄, 9-anthryl, 3,4-Cl₂C₆H₃, 3,4,5-(MeO)₃C₆H₂, piperonyl, nicotiny, 2-furyl, PhCH:CH] to give 20-70% RC:lpbond.CCH:CHR1. Addnl. obtained were 28% I and 35% II.

Hit Structure

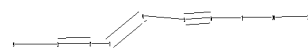
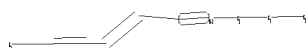
CAS Registry Number
77295-85-3 CAPLUS

Chemical or Trade Name
Benzene, 1,4-bis[4-(4-methylphenyl)-1-buten-3-ynyl]-, (E,E)- (9CI) (CA
INDEX NAME)



OS.CITING REF COUNT: 32 THERE ARE 32 CAPLUS RECORDS THAT CITE THIS
RECORD (32 CITINGS)

=>



chain nodes :
1 2 3 4 5 6 7 9 14 15
chain bonds :
1-2 1-9 2-3 3-4 4-5 5-6 6-7 7-14 14-15
exact/norm bonds :
1-9 6-7 7-14 14-15
exact bonds :
1-2 2-3 3-4 4-5 5-6

G1:Cb,Cy,Hy

G2:C,H,Si,Cb,Cy,Hy

G3:C,O,S,N

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:Atom 9:Atom 14:CLASS 15:Atom

L9 STRUCTURE UPLOADED

=> s 19 sss full
FULL SEARCH INITIATED 12:59:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 52774 TO ITERATE

100.0% PROCESSED 52774 ITERATIONS 101 ANSWERS
SEARCH TIME: 00.00.01

L10 101 SEA SSS FUL L9

=> s 110

L11 30 L10

=> 111 and (py<=2004 or ay<=2004)
25158915 PY<=2004
5170681 AY<=2004

L12 13 L11 AND (PY<=2004 OR AY<=2004)

=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 13 ANSWERS - CONTINUE? Y/(N):y

L12 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2001:398954 CAPLUS [Full-Text](#)

Document Number

135:164303

Title

Fluorescent fingerprinting of molecular recognition landscapes

Author/Inventor

Auer, Manfred; Graf, Christine; La Clair, James J.

Patent Assignee/Corporate Source

Allergic Diseases Unit Fluorescence based HTS-Technology Program, Novartis Forschungsinstitut GmbH, Vienna, 1235, Austria

Source

Angewandte Chemie, International Edition (2001), 40(10), 1889-1892 CODEN: ACIEF5; ISSN: 1433-7851

Document Type

Journal

Language

English

Abstract

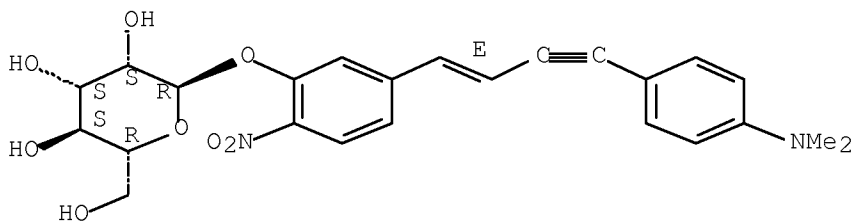
The combination of a non-ridges fluorescence probe (SENSI) and three-dimensional fluorescence spectroscopy provides an efficient means to differentiate subtle structural attributes resulting from mol. interactions. This method was able to distinguish low-affinity protein-carbohydrate interactions. The ease and tech. simplicity of this method suggest a practical means to increase the reliability of affinity matrixes, and illustrate a potent tool for characterizing (or landscaping) a wide-range of biol. and chemical processes (e.g. drug screening, characterization of chemical purity, and resolution of mixture). As seen here, it is not the affinity but the "fingerprint" of mol. recognition which is vital in selecting compds. for cellular and in vivo testing and for establishing structure-activity relationships for follow up bioinformatics, mol. modeling, and/or rational drug design. Most importantly, this three-dimensional method provides a means to distinguish recognition events from stoichiometric effects.

Hit Structure

CAS Registry Number
353521-92-3 CAPLUS

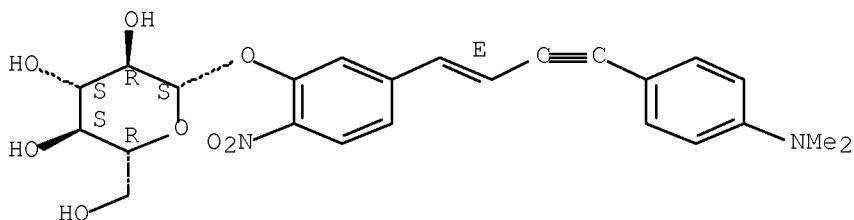
Chemical or Trade Name

α -D-Mannopyranoside, 5-[(1E)-4-[4-(dimethylamino)phenyl]-1-buten-3-ynyl]-2-nitrophenyl (9CI) (CA INDEX NAME)



CAS Registry Number
193957-48-1 CAPLUS

Chemical or Trade Name
 β -D-Glucopyranoside, 5-[(1E)-4-[4-(dimethylamino)phenyl]-1-buten-3-ynyl]-2-nitrophenyl (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

. L12 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2000:890415 CAPLUS [Full Text](#)

Document Number

134:252506

Title

Cross-coupling reactions in Cinchona alkaloid chemistry: aryl-substituted and dimeric quinine, quinidine, as well as quincorine and quincoridine derivatives

Author/Inventor

Frackepohl, Jens; Braje, Wilfried M.; Hoffmann, H. Martin R.

Patent Assignee/Corporate Source

Department of Organic Chemistry, Universitat Hannover, Hannover, D-30167, Germany

Source

Journal of the Chemical Society, Perkin Transactions 1 (2001), (1), 47-65 CODEN: JCSPCE; ISSN: 1472-7781

Document Type

Journal

Language

English

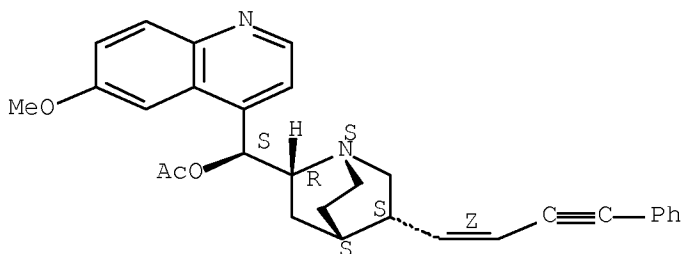
Abstract

Cross-coupling reactions of modified Cinchona alkaloids provide access to a wide variety of novel arylated and dimeric derivs. of quinine and quinidine containing a single and double 1,2-amino alc. functionality. Sonogashira and Heck reactions allow functionalization of ethynyl and 11-iodovinyl precursors. The role of bystander functionality is investigated.

Hit Structure

CAS Registry Number
331250-66-9 CAPLUS

Chemical or Trade Name
10,11-Dinorcinchonane-9-ol, 6'-methoxy-3-[(1Z)-4-phenyl-1-buten-3-ynyl]-, acetate (ester), (3 β ,9S)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 23 THERE ARE 23 CAPLUS RECORDS THAT CITE THIS
RECORD (23 CITINGS)

. L12 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

2000:768991 CAPLUS [Full Text](#)

Document Number

133:331792

Title
Fluorescent dye
Author/Inventor
Laclair, James J.
Patent Assignee/Corporate Source
The Scripps Research Institute, USA
Source
U.S., 36 pp., Cont-in-part of U.S. Ser. No. 17,518. CODEN: USXXAM
Document Type
Patent
Language
English
Patent Information

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6140041	A	20001031	US 1999-232356	19990115
US 5958673	A	19990928	US 1998-17518	19980202

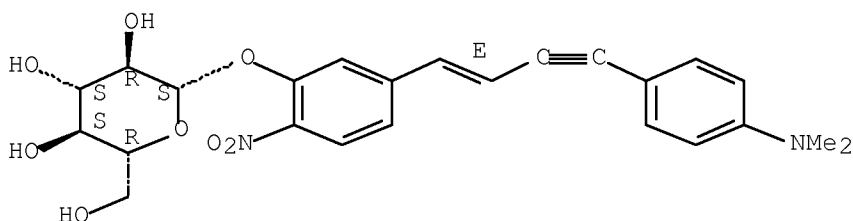
Abstract

Fluorescent dyes possess reactive linkers for conjugating to nucleic acids, carbohydrates and peptides. The conjugates fluoresce in the visible and UV spectrum and have an excellent solvchromatic response as compared to other fluorescence or chromatic labels. The conjugates are stable but also have medium sensitive. The fluorescent dyes have little triplet state formation and are not photoreactive, making them an excellent substance for biological investigations. Uses for the dyes include protein labeling, DNA labeling, single mol. spectroscopy and fluorescence. A synthesis of the dyes is disclosed. Methods of use include the detection of carbohydrate-protein interactions.

Hit Structure

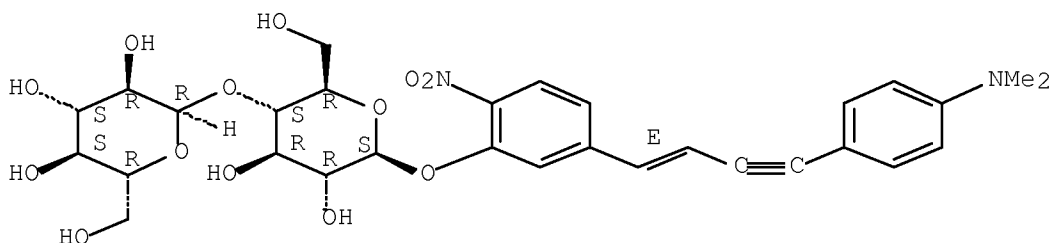
CAS Registry Number
193957-48-1 CAPLUS

Chemical or Trade Name
β-D-Glucopyranoside, 5-[(1E)-4-[4-(dimethylamino)phenyl]-1-buten-3-ynyl]-2-nitrophenyl (9CI) (CA INDEX NAME)



CAS Registry Number
235793-03-0 CAPLUS

Chemical or Trade Name
β-D-Glucopyranoside, 5-[(1E)-4-[4-(dimethylamino)phenyl]-1-buten-3-ynyl]-2-nitrophenyl 4-O-α-D-glucopyranosyl- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD
(6 CITINGS)

L12 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number
1999-686375 CAPLUS [Full-text](#)
Document Number
132:247772

Title
Screening hydrolysis over two-phases
Author/Inventor
Cotencescu, M.-G.; La Clair, J. J.
Patent Assignee/Corporate Source
Department of Molecular Biology, The Scripps Research Institute, La Jolla, CA, USA
Source
Journal of Biotechnology (1999), 76(1), 33-41 CODEN: JBITD4; ISSN: 0168-1656
Document Type
Journal
Language
English

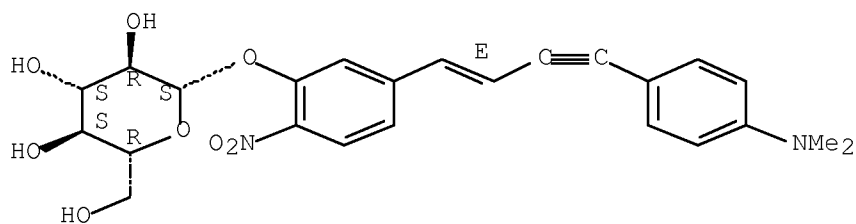
Abstract

A new assay is described that monitors hydrolysis with the concurrent transfer of a solvatochromic dye across an oil-water barrier. Through the appropriate design, this transfer is accompanied by a 106 gain in fluorescence. This response can be used to effectively screen hydrolytic activity at high-throughput. Using this method, microunits of alkaline phosphatase, glucosidases, as well as several common proteases can be visually detected within an hour through concentration over a 200:1 volumetric ratio of aqueous to organic phases. Development of a water-solubilizing protecting group extends this methodol. to screen a wide range of processes that undergo cleavage of a covalent bond.

Hit Structure

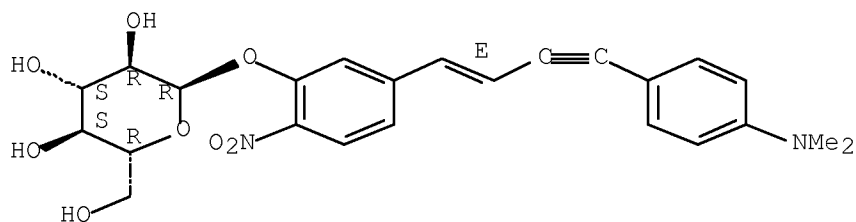
CAS Registry Number
193957-48-1 CAPLUS

Chemical or Trade Name
 β -D-Glucopyranoside, 5-[(1E)-4-[4-(dimethylamino)phenyl]-1-buten-3-ynyl]-2-nitrophenyl (9CI) (CA INDEX NAME)



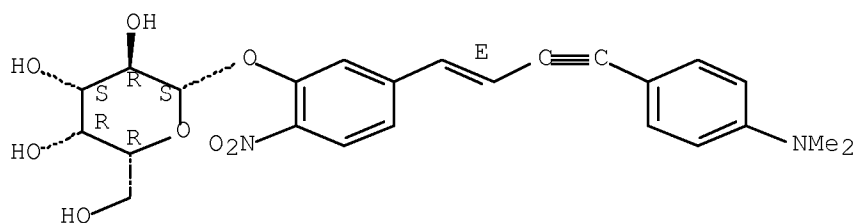
CAS Registry Number
262856-71-3 CAPLUS

Chemical or Trade Name
 α -D-Glucopyranoside, 5-[(1E)-4-[4-(dimethylamino)phenyl]-1-buten-3-ynyl]-2-nitrophenyl (9CI) (CA INDEX NAME)



CAS Registry Number
262856-72-4 CAPLUS

Chemical or Trade Name
 β -D-Galactopyranoside, 5-[(1E)-4-[4-(dimethylamino)phenyl]-1-buten-3-ynyl]-2-nitrophenyl (9CI) (CA INDEX NAME)



L12 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1999:495343 CAPLUS [Full-text](#)

Document Number

131:145690

Title

Fluorescent dyes and conjugates, their preparation and use

Author/Inventor

Laclair, James J.

Patent Assignee/Corporate Source

Novartis A.-G., Switz.; Novartis-Erfindungen Verwaltungsgesellschaft m.b.H.; The Scripps Research Institute

Source

PCT Int. Appl., 66 pp. CODEN: PIXXD2

Document Type

Patent

Language

English

Patent Information

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9938919	A1	19990805	WO 1999-EP598	19990129
US 5958673	A	19990928	US 1998-17518	19980202
AU 9924253	A	19990816	AU 1999-24253	19990129

Abstract

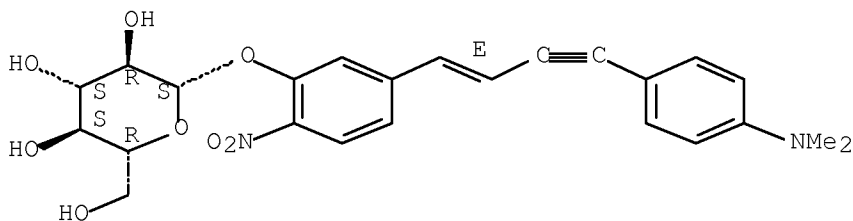
The fluorescent dyes I [R1 = 4-R3-1-piperazinyl, NR4R5; R2, R3 = H, COCH2nCO2R6, COR7; R4, R5 = C1-6 alkyl; R6 = C1-6 alkyl, succinimido; R7 = 1-imidazolyl, OCMn3; n = 1-4] possess reactive linkers for conjugating to nucleic acids, carbohydrates and peptides. The conjugates fluoresce in the visible and UV spectrum and show a greater solvatochromic response than other fluorescence or chromatic labels. The conjugates are stable but also medium sensitive. The fluorescent dyes have little triplet state formation and are not photoreactive, making them suitable for biol. investigations. Uses for the dyes include protein labeling, DNA labeling, single mol. spectroscopy and fluorescence. Thus, 3-hydroxy-4-nitrobenzaldehyde was reduced to the corresponding benzyl alc., converted to the bromide and then to the di-Et phosphonate, and treated with 4-R1C6H4C.tpbond.CCHO to give I (R2 = H).

Hit Structure

CAS Registry Number
193957-48-1 CAPLUS

Chemical or Trade Name

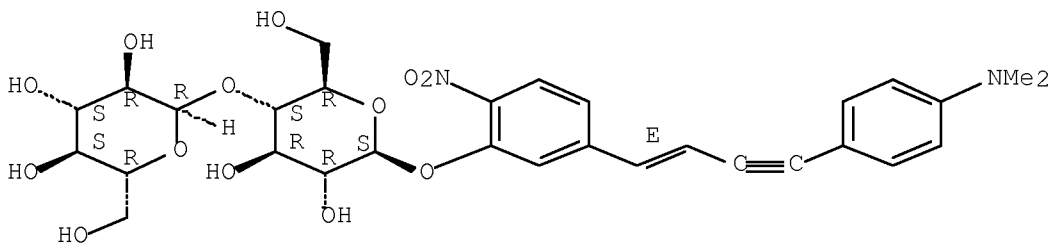
β -D-Glucopyranoside, 5-[(1E)-4-[4-(dimethylamino)phenyl]-1-buten-3-ynyl]-2-nitrophenyl (9CI) (CA INDEX NAME)



CAS Registry Number
235793-03-0 CAPLUS

Chemical or Trade Name

β -D-Glucopyranoside, 5-[(1E)-4-[4-(dimethylamino)phenyl]-1-buten-3-ynyl]-2-nitrophenyl 4-O- α -D-glucopyranosyl- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L12 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1999:133455 CAPLUS [Full-text](#)

Document Number

130:210546

Title

The photoconductive composition containing a 1,4-diphenyl-1-butyne-3-ene derivative as electron donor

Author/Inventor

Chung, Bong-Mo; Suk, Min-Chul; Shim, Sang-Chul

Patent Assignee/Corporate Source

Samsung Electron Devices Co., Ltd., S. Korea

Source

Jpn. Kokai Tokkyo Koho, 11 pp. CODEN: JKXXAF

Document Type

Patent

Language

Japanese

Patent Information

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11049968	A	19990223	JP 1998-160883	19980609
JP 2897985	B2	19990531		
US 5989766	A	19991123	US 1998-93058	19980608
CN 1221132	A	19990630	CN 1998-116092	19980717

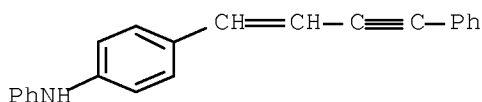
Abstract

Photoconductive composition for photoconductive film having excellent sensitivity and thermal deposition property comprises a 1,4-diphenyl-1-butyne-3-ene derivative as electron donor, an electron acceptor, a charge-transfer compound, binder, a surfactant, and a solvent. Thus the interior panel of a cathode ray tube was coated with a conductive coating, then a photoconductive coating comprising 1,4-diphenyl-1-butyne-3-ene 25, 2,4-dinitroaniline 2.5, triphenylamine 25, polystyrene 250, silica 1000.1 and toluene 2595 g, followed by attaching green, red and blue fluorescent composition and IR heat melting to give a fluorescent tube.

Hit Structure

CAS Registry Number
220929-00-0 CAPLUS

Chemical or Trade Name
Benzenamine, N-phenyl-4-(4-phenyl-1-buten-3-yn-1-yl)- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD
(1 CITINGS)

L12 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number
1997:528726 CAPLUS [Full Text](#)
Document Number
127:176623

Title

Selective Detection of the Carbohydrate-Bound State of Concanavalin A at the Single Molecule Level

Author/Inventor

La Clair, James J.

Patent Assignee/Corporate Source

Department of Molecular Biology, Scripps Research Institute, La Jolla, CA, 92037, USA

Source

Journal of the American Chemical Society (1997), 119(33), 7676-7684 CODEN: JACSAT; ISSN: 0002-7863

Document Type

Journal

Language

English

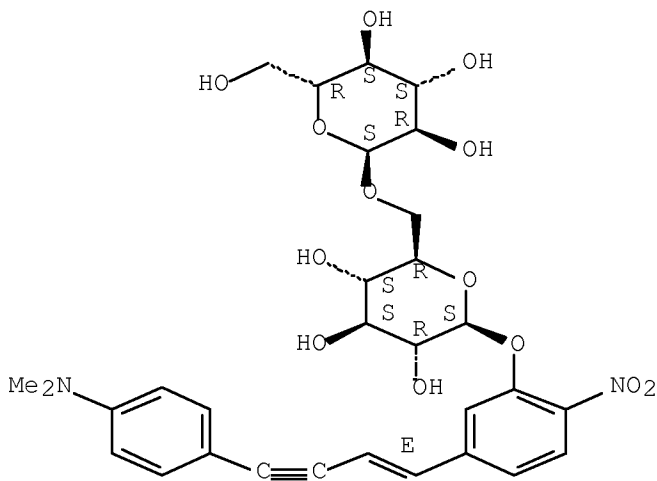
Abstract

The labeling of mols. with charge-transfer dyes, such as dansyl chloride, is a powerful tool for examining the solvent shell of attached substances. This investigation describes the synthesis and application of a new charge transfer label based on (E,E)-4-O-2NC6H4CH:CHCH:CHC6H4NMe2-4 (NND). Unlike many commonly used fluorophores, the quantum yield of NND decreases over 4 orders of magnitude upon changing from nonpolar to polar environments. In addition, several derivs. of NND undergo little photodecompn. and can be detected at the picomolar level in a confocal fluorescence correlation spectrometer. In conjunction with recent detection of single mols. in solution, this paper describes a method to discriminate between single free and carbohydrate-bound aggregates of the Jack Bean lectin, Con A. To this end, two NND derivs. were constructed possessing an addnl. functional handle. One derivative, alkenyne (E)-3,4-HO(NO2)C6H4CH:CHC.tpbond.CC6H4NMe2-4 (I), was efficiently attached to the β -anomeric position of glucopyranosides. Transients from single aggregates of this fluorophore were detected in solns. which contained both Con A and a maltoside conjugate of I, and not the corresponding glucoside conjugate of I. This result is in agreement with the known affinity of Con A for α -glucopyranosides and not β -glucopyranosides. A full description of the synthesis of these dyes, their solvchromatic properties, and the method used for single aggregate detection is provided.

Hit Structure

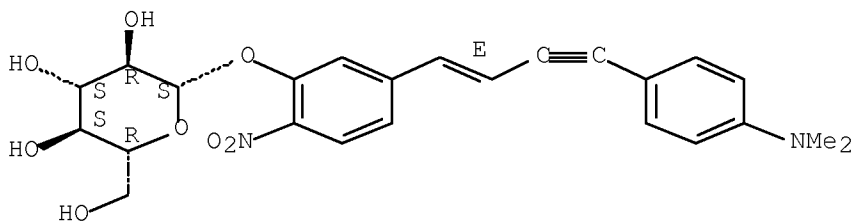
CAS Registry Number
193957-47-0 CAPLUS

Chemical or Trade Name
 β -D-Glucopyranoside, 5-[(1E)-4-[4-(dimethylamino)phenyl]-1-buten-3-ynyl]-2-nitrophenyl 6-O- α -D-glucopyranosyl- (9CI) (CA INDEX NAME)



CAS Registry Number
193957-48-1 CAPLUS

Chemical or Trade Name
 β -D-Glucopyranoside, 5-[[1(E)-4-[4-(dimethylamino)phenyl]-1-buten-3-ynyl]-2-nitrophenyl (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 19 THERE ARE 19 CAPLUS RECORDS THAT CITE THIS RECORD (19 CITINGS)

. L12 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1997:383287 CAPLUS [Full-text](#)

Document Number

127:109010

Title

Reactions of the phenyl-substituted five-membered titanacyclocumulene - unusual coupling of a 1,4-disubstituted 1,3-butadiyne with two titanium atoms

Author/Inventor

Burlakov, Vladimir V.; Peulecke, Norman; Baumann, Wolfgang; Spannenberg, Anke; Kempe, Rhett; Rosenthal, Uwe

Patent Assignee/Corporate Source

Arbeitsgruppe Komplexkatalyse of the Max-Planck-Gesellschaft at the University of Rostock, Buchbinderstr. 5-6, D-18055, Rostock, Germany

Source

Journal of Organometallic Chemistry (1997), 536/537(1-2), 293-297 CODEN: JORCAI; ISSN: 0022-328X

Document Type

Journal

Language

English

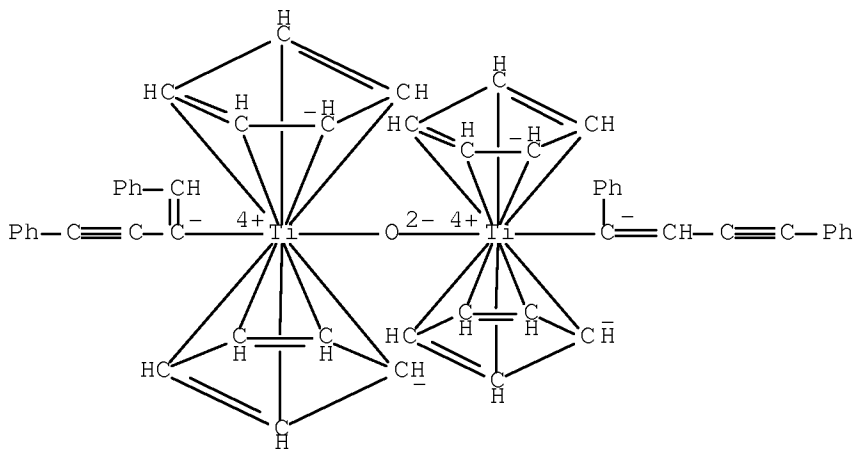
Abstract

The reaction of $\text{Cp}_2\text{Ti}(\eta^2\text{-Me}_3\text{SiC}_2\text{SiMe}_3)$ with equimolar amts. of $\text{PhC}\equiv\text{C-C}\equiv\text{C-Ph}$ gives the unstable five-membered titanacyclocumulene I, which is stabilized by dimerization to yield the dinuclear complex II. In this reaction complex I shows an equilibrium and also behaves as a metallacyclocumulene and a metal alkyne complex. By the coupling of the internal double bond of the cyclocumulene with a complexed triple bond of the diyne, a complex with fused titanacyclopentadiene and titanacyclopentene is formed. With acetone and water complex I reacts like an alkyne complex to give the titanadhydroturan III and the titanoxane IV. Complex II was investigated by an X-ray structural determination

Hit Structure

CAS Registry Number
192374-58-6 CAPLUS

Chemical or Trade Name
Titanium, tetrakis(η^5 -2,4-cyclopentadien-1-yl) (1,4-diphenyl-1-buten-3-ynyl)- μ -oxo[3-phenyl-1-(phenylmethylene)-2-propynyl]di-, (E,E)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

L12 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1981:157334 CAPLUS [Full-text](#)

Document Number

94:157334

Title

Synthesis and properties of conjugated enyne polysulfones

Author/Inventor

Reinhardt, Bruce A.; Arnold, Fred E.

Patent Assignee/Corporate Source

Nonmetallic Mater. Div., Air Force Mater. Lab., Wright-Patterson Air Force Base, OH, 45433, USA

Source

Journal of Polymer Science, Polymer Chemistry Edition (1981), 19(2), 271-85 CODEN: JPLCAT; ISSN: 0360-6376

Document Type

Journal

Language

English

Abstract

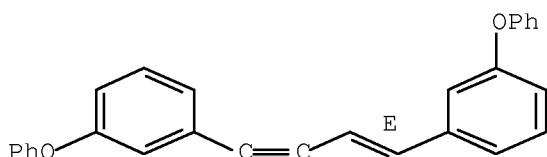
High-mol.-weight polysulfones containing 1,3-enyne linkages were prepared from K salts of (E)-1,4-bis(3-hydroxyphenyl)-1-buten-3-yne [76410-52-1] and 4,4'-dihydroxybiphenyl with bis(4-halophenyl) sulfones in DMSO-sulfolane. The polymers were soluble in CH₂Cl₂ and had intrinsic viscosities ≤ 0.74 (AcNMe₂, 30°) and glass transition temps. 179-214°. Thermal anal. of cured films and of products of thermal reactions of model compds. indicated that the primary curing reaction was intermol. rather than the expected intramol. cycloaddn. to naphthalene derivs. The enyne polysulfones are suitable for use in high-temperature composites.

Hit Structure

CAS Registry Number
77214-78-9 CAPLUS

Chemical or Trade Name

Benzene, 1,1'-(1-buten-3-yne-1,4-diyl)bis[3-phenoxy-, (E)- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 4 THERE ARE 4 CAPLUS RECORDS THAT CITE THIS RECORD
(4 CITINGS)

L12 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1979:557429 CAPLUS [Full-text](#)

Document Number

91:157429

Title

Aromatic enyne compounds

Author/Inventor

Arnold, Fred E.; et al.

Patent Assignee/Corporate Source

United States Dept. of the Air Force, USA

Source

U. S. Pat. Appl., 14 pp. Avail. NTIS. CODEN: XAXXAV

Document Type

Patent

Language

English

Patent Information

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 946290	A0	19790427	US 1978-946290	19780927
US 4162265	A	19790724	US 1978-946290	19780927

Abstract

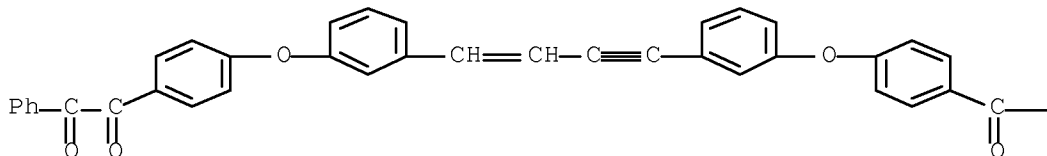
RC₆H₄CH:CHC.tplbond.CC₆H₄R (I, R = OH, NH₂, 4-PhCOCOC₆H₄O or other functional group suitable for polycondensation reactions), useful as monomers for thermal polymerization (no data), were prepared by catalytic coupling of RC₆H₄C.tplbond.CH. Thus, 3-H₂NC₆H₄C.tplbond.CH was acetylated, coupled by refluxing 12 h with AcOCu in AcOH, then deacetylated by refluxing 1 h in 28% aqueous EtOH to give I (R = 3-NH₂).

Hit Structure

CAS Registry Number
70933-63-0 CAPLUS

Chemical or Trade Name

Ethanedione, 1,1'-(1-buten-3-yne-1,4-diylbis(3,1-phenyleneoxy-4,1-phenylene))bis[2-phenyl- (9CI) (CA INDEX NAME)



PAGE 1-A

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4162265	A	19790724	US 1978-946290	19780927
US 946290	A0	19790427	US 1978-946290	19780927

Chemical or Trade Name
Ethanedione, 1,1'-[1-buten-3-yne-1,4-diylbis(3,1-phenyleneoxy-4,1-phenylene)]bis[2-phenyl- (9CI) (CA INDEX NAME)

O=C(c1ccc(Oc2ccc(C=CC#Cc3ccc(Oc4ccc(C(=O)c5ccccc5)cc4)cc3)cc2)cc1)c6ccccc6
$$\text{---C(=O)Ph}$$

Abstract

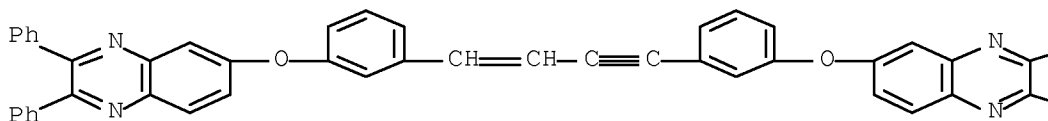
[3-(3,4-Diaminophenoxy)phenyl]acetylene [58297-25-9]-terminated oligomeric poly(phenylquinoxalines) were soluble (20-30%) in low-boiling organic solvents and exhibited a high degree of flow at their softening temps. Thermal anal. data obtained on the oligomers indicated initial softening at approx. 160 and a strong polymerization exotherm reaching a maximum at 274°. Cured polymers (8 h, 280°) exhibited glass-transition temps. at approx. 320°. Mass spectrometry-thermogravimetry of the polymers showed that no volatiles were emitted during curing and that decomposition of the resins began at 465°.

Hit Structure

CAS Registry Number
63389-28-6 CAPLUS

Chemical or Trade Name
Quinoxaline, 6,6'-[1-buten-3-yne-1,4-diylbis(3,1-phenyleneoxy)]bis[2,3-diphenyl- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



OS.CITING REF COUNT: 20 THERE ARE 20 CAPLUS RECORDS THAT CITE THIS RECORD (20 CITINGS)

_L12 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2010 ACS on STN

Accession Number

1962:79498 CAPLUS [Full-text](#)

Document Number

56:79498

Title

Possible use of betaine-like methylenetriphenylphosphoranes as reagents for characterization of aldehydes. II. Preparation of characteristic derivatives

Author/Inventor

Simalty-Siemiatycki, Michel; Malbec, Francoise; Carretto, Josette

Patent Assignee/Corporate Source

Fac. Sci., Paris

Source

Bulletin de la Societe Chimique de France (1962) 129-31 CODEN: BSCFAS; ISSN: 0037-8968

Document Type

Journal

Language

Unavailable

Abstract

For the preparation of characteristic derivs. of aldehydes, the use of excess reagent, absolute alc. as solvent, and NaOEt as base is recommended. In some cases dilution of the alc. up to 50% with H2O is necessary. For differentiation of aldehydes from ketones, alc. containing 5-10% H2O is used as solvent. Derivs. prepared from II are preferred since they are less soluble and have higher m.p. than those prepared from I. Acrolein and α -ethylacrolein gave oils. The bisulfite addition product of glyoxal was used, with excess NaOEt to neutralize the bisulfite; even with less reagent than that corresponding to 1 CHO group, a disubstituted derivative was obtained. The stereochem. configuration of the derivs. was determined by infrared and Raman spectra. The following derivs. of I and II were prepared [aldehyde, reagent, m.p., and color (if other than white) given]: (CH2O)3, I, 89.5°; (CH2O)3, II, 132.5°; IV, II, 105-6°; V, II, 115-18°; C6H13CHO, I, 103.5°; XVI, II, 164-6°, pale yellow; VII, II, 179-81°; (OHC)2, II, (disubstituted derivs.) trans-trans 313°, cis-cis 300°, both yellow; HO2CCHO, II, 159°; VIII, II, trans 142-3°, pale yellow; X, II, 169-71°; III, I, 211-12°; pale green; III, II, 239-40°; pale green; XI, II, 210-11°; Ph2C=CHCHO, II, 202.5°; 9-fluorenylideneacetaldehyde, II, 218°, yellow; MePhC=CHCH:CHCHO, II, 167°, yellow; XII, II, 233-3.5°; XIII, II, 188.5°; XIV, I, 159°; XV, II, 252°; o-PhC6H4CHO (XVII), I, 182.5°; XVII, II, 174°; p-MeOC6H4CHO, II, 228.5°; piperonal, II, 205-6°; m-O2NC6H4CHO, II, trans 188-9°; cis 112-13°; both yellow; p-O2NC6H4CHO, II, 232.5°, yellow; p-Me2NC6H4CHO, II, 295°, yellow; furfural, II, 237°; 2-thiophenecarboxaldehyde, II, 241°, yellow; 5-nitro-2-thiophenecarboxaldehyde, II, 278°, yellow-green.

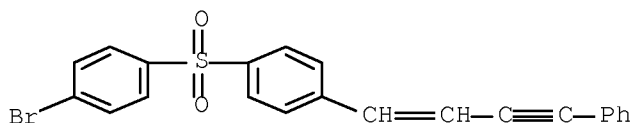
Hit Structure

CAS Registry Number

96065-74-6 CAPLUS

Chemical or Trade Name

Benzene, 1-[[(4-bromophenyl)sulfonyl]-4-(4-phenyl-1-buten-3-yn-1-yl)]- (CA INDEX NAME)



=>

---Logging off of STN---

=>

Executing the logoff script...